January 1984

ISSN 0301-0104

Chemical Physics

A journal devoted to experimental and theoretical research involving problems of both a chemical and physical nature

UNIVERSITY OF HAWAII
LIBRARY
MAR 22 6 56 AM '84

MASTER INDEX

VOLUMES 71–80

SEPTEMBER 1982–OCTOBER 1983

Editors

ROBIN M. HOCHSTRASSER/G. LUDWIG HOFACKER

RIODICAL
D
50
44
80
Index
H. LIBRARY

CHEMICAL PHYSICS

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

EDITORS

ROBIN M. HOCHSTRASSER
Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA

G. LUDWIG HOFACKER
Lehrstuhl für Theoretische Chemie, Technische Universität München, Lichtenbergstrasse 4, 8046 Garching near Munich, Germany

ADVISORY EDITORIAL BOARD

Australia
R.D. BROWN, Clayton, Victoria
D.P. CRAIG, F.R.S., Canberra
N.S. HUSH, Sydney
J.D. MORRISON, Bundoora, Victoria

Belgium
J. DUCHESNE, Liège

Canada
G.W. KING, Hamilton, Ontario
J.A. KONINGSTEIN, Ottawa
T. OKA, Ottawa
J.C. POLANYI, F.R.S., Toronto

Czechoslovakia
Z. HERMAN, Prague

Denmark
T.A. BAK, Copenhagen
J. LINDERBERG, Aarhus

Federal Republic of Germany
S.F. FISCHER, Munich
W. KAISER, Munich
D. MENZEL, Garching
E.W. SCHLAG, Munich
J.P. TOENNIES, Göttingen
H.C. WOLF, Stuttgart

France
S. LEACH, Orsay
J.-C. LEHMANN, Paris
A. TRAMER, Orsay

German Democratic Republic
L. ZÜLICKE, Berlin

Israel
J. JORTNER, Tel Aviv
R.D. LEVINE, Jerusalem
S. LIFSON, Rehovot

Italy
M. CAPITELLI, Bari
G. CARERI, Rome

Japan
N. MATAGA, Osaka
S. NAGAKURA, Okazaki
K. YOSHIHARA, Okazaki

Jugoslavia
R. BLINC, Ljublijana

The Netherlands
J. KISTEMAKER, Amsterdam
J. LOS, Amsterdam
J. REUSS, Nijmegen

New Zealand
L.F. PHILLIPS, Christchurch

Norway
R. MANNE, Bergen

Poland
A. WITKOWSKI, Cracow

Sweden
E. LINDHOLM, Stockholm
K. SIEGBAHN, Uppsala

Switzerland
H. FISCHER, Zurich
Hs.H. GÜNTHARD, Zurich
J.P. MAIER, Basel

United Kingdom
A.D. BUCKINGHAM, F.R.S., Cambridge
A.B. CALLEAR, Cambridge
A. CARRINGTON, Southampton
W.C. PRICE, London

USA
J.M. DEUTCH, Cambridge, MA
M.A. EL-SAYED, Los Angeles, CA
M.E. FISHER, Ithaca, NY
G. FLYNN, New York, NY
F.K. FONG, Lafayette, IN
K.F. FREED, Chicago, IL
W.A. GODDARD III, Pasadena, CA
D.M. HANSON, Stony Brook, NY
C.B. HARRIS, Berkeley, CA
K.K. INNES, Binghamton, NY
M. KASHA, Tallahassee, FL
W. KLEMPERER, Cambridge, MA
W.C. LINEBERGER, Boulder, CO
D.S. McCLURE, Princeton, NJ
J.D. McDONALD, Urbana, IL
R.E. MERRIFIELD, Wilmington, DE
W.H. MILLER, Berkeley, CA
D.W. OXTOBY, Chicago, IL
C.S. PARMENTER, Bloomington, IN
W. PLUMMER, Philadelphia, PA
J.A. POPLE, Pittsburgh, PA
P.M. RENTZEPIS, Murray Hill, NJ
G.W. ROBINSON, Lubbock, TX
D.H. SECREST, Urbana, IL
R.N. ZARE, Stanford, CA
R.W. ZWANZIG, College Park, MD

USSR
A.I. BURSHTEIN, Novosibirsk
V.S. LETOKHOV, Moscow
N.N. SEMENOV, Moscow
V.L. TALROSE, Moscow

Chemical Physics is published semi-monthly. The 1984 subscription price per volume is Dfl. 245.00 (approx. $ 98.00) excluding Dfl. 21.00 (approx. $ 8.50) postage and handling. Claims for issues not received should be made within three months of publication. If not, they cannot be honoured free of charge.

Subscriptions should be sent to the publisher: ELSEVIER SCIENCE PUBLISHERS B.V., Journals Department, P.O. Box 211, 1000 AE Amsterdam, The Netherlands, or to any subscription agent or bookseller.

Elsevier Science Publishers B.V. All rights reserved. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior permission of the publisher, Elsevier Science Publishers B.V. (North-Holland Physics Publishing Division), P.O. Box 103, 1000 AC Amsterdam, The Netherlands.

Special regulations for authors. Upon acceptance of an article by the journal, the author(s) will be asked to transfer copyright of the article to the publisher. This transfer will ensure the widest possible dissemination of information.

Submission to this journal of a paper entails the author's irrevocable and exclusive authorization of the publisher to collect any sums or considerations for copying or reproduction payable by third parties (as mentioned in article 17 paragraph 2 of the Dutch Copyright Act of 1912 and in the Royal Decree of June 20, 1974 (S.351) pursuant to article 16b of the Dutch Copyright Act of 1912) and/or to act in or out of Court in connection therewith.

Special regulations for readers in the USA. This journal has been registered with the Copyright Clearance Center, Inc. Consent is given for copying of articles for personal or internal use, or for the personal use of specific clients. This consent is given on the condition that the copier pays through the Center the per-copy fee stated in the code on the first page of each article for copying beyond that permitted by Sections 107 and 108 of the US Copyright Law. The appropriate fee should be forwarded with a copy of the first page of the article to the Copyright Clearance Center, Inc., 21 Congress Street, Salem, MA 01970, USA. If no code appears in an article, the author has not given broad consent to copy and permission to copy must be obtained directly from the author. All articles published prior to 1981 may be copied for a per-copy fee of US $ 2.25, also payable through the Center. This consent does not extend to other kinds of copying, such as for general distribution, resale, advertising and promotion purposes, or for creating new collective works. Special written permission must be obtained from the publisher for such copying.

Printed in The Netherlands

Published semi-monthly

CHEMICAL PHYSICS

CHEMICAL PHYSICS

A journal devoted to experimental and theoretical research involving problems of both a chemical and a physical nature

EDITORS

ROBIN M. HOCHSTRASSER
Department of Chemistry, University of Pennsylvania,
Philadelphia, PA 19104, USA

G. LUDWIG HOFACKER
Lehrstuhl für Theoretische Chemie, Technische Universität München,
Lichtenbergstrasse 4, 8046 Garching near Munich, Germany

ADVISORY EDITORIAL BOARD

Australia
R.D. BROWN, Clayton, Victoria
D.P. CRAIG, F.R.S., Canberra
N.S. HUSH, Sydney
J.D. MORRISON, Bundoora, Victoria

Belgium
J. DUCHESNE, Liège

Canada
G.W. KING, Hamilton, Ontario
J.A. KONINGSTEIN, Ottawa
T. OKA, Ottawa
J.C. POLANYI, F.R.S., Toronto

Czechoslovakia
Z. HERMAN, Prague

Denmark
T.A. BAK, Copenhagen
J. LINDERBERG, Aarhus

Federal Republic of Germany
S.F. FISCHER, Munich
W. KAISER, Munich
D. MENZEL, Garching
E.W. SCHLAG, Munich
J.P. TOENNIES, Göttingen
H.C. WOLF, Stuttgart

France
S. LEACH, Orsay
J.-C. LEHMANN, Paris
A. TRAMER, Orsay

German Democratic Republic
L. ZÜLICKE, Berlin

Israel
J. JORTNER, Tel Aviv
R.D. LEVINE, Jerusalem
S. LIFSON, Rehovot

Italy
M. CAPITELLI, Bari
G. CARERI, Rome

Japan
N. MATAGA, Osaka
S. NAGAKURA, Okazaki
K. YOSHIHARA, Okazaki

Jugoslavia
R. BLINC, Ljublijana

The Netherlands
J. KISTEMAKER, Amsterdam
J. LOS, Amsterdam
J. REUSS, Nijmegen

New Zealand
L.F. PHILLIPS, Christchurch

Norway
R. MANNE, Bergen

Poland
A. WITKOWSKI, Cracow

Sweden
E. LINDHOLM, Stockholm
K. SIEGBAHN, Uppsala

Switzerland
H. FISCHER, Zurich
Hs.H. GÜNTHARD, Zurich
J.P. MAIER, Basel

United Kingdom
A.D. BUCKINGHAM, F.R.S., Cambridge
A.B. CALLEAR, Cambridge
A. CARRINGTON, Southampton
W.C. PRICE, London

USA
J.M. DEUTCH, Cambridge, MA
M.A. EL-SAYED, Los Angeles, CA
M.E. FISHER, Ithaca, NY
G. FLYNN, New York, NY
F.K. FONG, Lafayette, IN
K.F. FREED, Chicago, IL
W.A. GODDARD III, Pasadena, CA
D.M. HANSON, Stony Brook, NY
C.B. HARRIS, Berkeley, CA
K.K. INNES, Binghamton, NY
M. KASHA, Tallahassee, FL
W. KLEMPERER, Cambridge, MA
W.C. LINEBERGER, Boulder, CO
D.S. McCLURE, Princeton, NJ
J.D. McDONALD, Urbana, IL
R.E. MERRIFIELD, Wilmington, DE
W.H. MILLER, Berkeley, CA
D.W. OXTOBY, Chicago, IL
C.S. PARMENTER, Bloomington, IN
W. PLUMMER, Philadelphia, PA
J.A. POPLE, Pittsburgh, PA
P.M. RENTZEPIS, Murray Hill, NJ
G.W. ROBINSON, Lubbock, TX
D.H. SECREST, Urbana, IL
R.N. ZARE, Stanford, CA
R.W. ZWANZIG, College Park, MD

USSR
A.I. BURSHTEIN, Novosibirsk
V.S. LETOKHOV, Moscow
N.N. SEMENOV, Moscow
V.L. TALROSE, Moscow

CHEMICAL PHYSICS

Editors

ROBIN M. HOCHSTRASSER, Philadelphia

G. LUDWIG HOFACKER, Munich

MASTER INDEX

VOLUMES 71–80 SEPTEMBER 1982–OCTOBER 1983

NORTH-HOLLAND PHYSICS PUBLISHING – AMSTERDAM

© Elsevier Science Publishers B.V. (North-Holland Physics Publishing Division) 1984

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior permission of the publisher, Elsevier Science Publishers B.V. (North-Holland Physics Publishing Division), P.O. Box 103, 1000 AC Amsterdam, The Netherlands.

Special regulations for authors. *Upon acceptance of an article by the journal, the author(s) will be asked to transfer copyright of the article to the publisher. This transfer will ensure the widest possible dissemination of information.*

Submission to this journal of an article entails the author's irrevocable and exclusive authorization of the publisher to collect any sums or considerations for copying or reproduction payable by third parties (as mentioned in article 17 paragraph 2 of the Dutch Copyright Act of 1912 and in the Royal Decree of June 20, 1974 (S.351) pursuant to article 16b of the Dutch Copyright Act of 1912) and/or to act in or out of Court in connection therewith.

Special regulations for readers in the USA. *This journal has been registered with the Copyright Clearance Center, Inc. Consent is given for copying of articles for personal or internal use, or for the personal use of specific clients. This consent is given on the condition that the copier pays through the Center the per-copy fee stated in the code on the first page of each article for copying beyond that permitted by Sections 107 or 108 of the US Copyright Law. The appropriate fee should be forwarded with a copy of the first page of the article to the Copyright Clearance Center, Inc., 21 Congress Street, Salem, MA 01970, USA. If no code appears in an article, the author has not given broad consent to copy and permission to copy must be obtained directly from the author. All articles published prior to 1981 may be copied for a per-copy fee of US $ 2.25, also payable through the Center. This consent does not extend to other kinds of copying, such as for general distribution, resale, advertising and promotion purposes, or for creating new collective works. Special written permission must be obtained from the publisher for such copying.*

PRINTED IN THE NETHERLANDS

CONTENTS

Author index to volumes 71–80 1

Subject index to volumes 71–80 45

Methods *45*

Theoretical *45*
Group theory and algebras 45
Classical mechanics and field theory 45
Stationary wavefunctions 45
Coupling schemes 48
Transport and relaxation theory 48
Statistical mechanics of equilibrium and stationary states 49
Thermodynamics and hydrodynamics 50
Many-body approaches 50
Collective excitations and quasiparticles 51
Computational methods 51
Theory of dynamics and scattering 54

Experimental *56*
Magnetic and electric resonance 56
Microwave spectroscopy 57
Infrared and Raman spectroscopy 57
Visible and ultraviolet spectroscopy 59
Photoelectron and ESCA spectroscopy 62
Double resonance spectroscopy 63
Lasers 63
Polarized light 65
Atomic and molecular beams 65
Time-resolved experiments 67
Cyclotron resonance 69
Mass spectra 69
Radiolysis 69
Mössbauer spectroscopy 69
Diffraction 70
P–V–T dependence 70
Scattering 70

Objects *71*

Bulk systems *71*
Gases 71
Liquids 73
Solutions 74
Crystals 75
Glasses and liquid crystals 78
Metals 78
Semiconductors 78
Surfaces 79
Dielectrics 79
Plasmas 79

Microscopic systems *80*
atoms 80
Molecules 81
Free radicals 88
Excitons 90
Defects and impurities 91
Ions and complexes 91
Dimers and molecular clusters 93
Polymers and biological macromolecules 94

Phenomena *94*

Atomic and molecular structure 94
Energy levels 98
Electric and magnetic properties 101
Spectral bandshapes and intensities 103
Relaxation phenomena 105
Energy transfer and conversion 108
Reactions 111
Intermolecular interactions 113
Ionic and excited state phenomena 116
Ionization 117
Isotope effects 119
Surface effects 119
Optical activity 120
Nonlinear optical effects 120
Field anisotropy 120
Transport of charge and mass 120
Thermodynamic properties 120
Structure of solids and liquids 121
Phase transitions 121

AUTHOR INDEX TO VOLUMES 71–80

Aarts, J.F.M., see J. Perrin 80 (1983) 351

Abed, S., M. Broyer, M. Carré, M.L. Gaillard and M. Larzillière, High-resolution spectroscopy of N_2O^+ in the near ultraviolet using FIBLAS (fast-ion-beam laser spectroscopy) 74 (1983) 97

Abramczyk, H., see W. Reimschüssel 72 (1982) 313

Achiba, Y., see S. Tomoda 74 (1983) 113

Adams, H.M., see D.K. Evans 80 (1983) 379

Addison, M., see T.A. Watson 78 (1983) 57

Aerts, F., see P. Willems 71 (1982) 27

Agarwal, U.P., R.S. Green and J. Yarwood, Vibrational relaxation of hydrogen-bonded species in solution. IV. Temperature and concentration dependence of the ν_σ(OH---N) band of phenol–pyridine 74 (1983) 35

Agmon, N., Local normal modes and vibrational adiabatic potentials 76 (1983) 203

Agostini, G., C. Corvaja, G. Giacometti and L. Pasimeni, Delayed-fluorescence ODMR and EPR studies of triplet excitons in charge-transfer molecular crystals 77 (1983) 233

Ågren, H., see P.-Å. Malmquist 76 (1983) 429

Ahlrichs, R. and P.R. Taylor, The structure of F_2O_2: theoretical predictions and comparisons with F_2 and F_2O 72 (1982) 287

Al Adel, F., L. Doyennette, M. Margottin-Maclou and L. Henry, Vibrational relaxation of $CO_2(00^01)$ and $N_2O(00^01)$ by NO 74 (1983) 413

Alfano, R.R., see Z.X. Yu 79 (1983) 289

Alford, P.C., C.G. Cureton, R.A. Lampert and D. Phillips, Fluorescence quenching of tertiary amines by halocarbons 76 (1983) 103

Allen, D.C. and C.J.S.M. Simpson, Rate constants for vibrational energy transfer between CO (v = 1) and CH_4 and substituted methane molecules in the temperature range 300 to 80 K 76 (1983) 231

Allnatt, A.R., see R.A. Aziz 78 (1983) 295

Alonso, J.A. and N.H. March, Density functional estimates of charge transfer and chemical potentials in hydrogen halides and mixed halides 76 (1983) 121

Al-Shamma, S.H., see I. Reineck 78 (1983) 311

Amat, G., On the use of "effective harmonic potentials" and "effective normal coordinates" in computing the vibrational energy level of polyatomic molecules 71 (1982) 363

Amirav, A., see G. Smulevich 73 (1982) 1

Amirav, A., see G. Smulevich 76 (1983) 147

Ancian, B., B. Tiffon and J.-E. Dubois, Molecular interactions and reorientational motion of neat acetone in the liquid state. ^{17}O NMR chemical shifts and linewidths at variable temperature 74 (1983) 171

Anglister, J. and I.Z. Steinberg, Resonance Rayleigh light scattering of some porphyrins in solution: intensities and depolarization ratios 75 (1983) 443

Anisimov, O.A., see A.B. Doktorov 71 (1982) 1

Aoiz, F.J., M.M. Oprysko and R.B. Bernstein, Argon ion laser excitation of supersonic seeded molecular beams of I_2 79 (1983) 321

Aoiz, F.J., see M.M. Oprysko 79 (1983) 341
Archirel, P. and P. Habitz, Surface hopping trajectory calculations for electronic rotational and vibrational inelastic collisions for the Na–N_2 system 78 (1983) 213
Argyrakis, P. and R. Kopelman, Dynamics of energy transport in ternary molecular solids. II. Time evolution of naphthalene fluorescence 78 (1983) 251
Arrowsmith, P., S.H.P. Bly, P.E. Charters, P. Chevrier, J.C. Polanyi and H.H. Telle, Collisional and radiational energy transfer in the system $Na^*(3\,^2P) + Na_2\,(X\,^1\Sigma^+) \rightarrow Na\,(3^2S) + Na_2^*\,(A\,^1\Sigma^+)$ 79 (1983) 31
Astruc, J.P., R. Barbé, A. Lagrèze and J.P. Schermann, Internal energy dependence of the autodetachment and dissociation times of the SF_6^- ion 75 (1983) 405
Avramides, E. and T.F. Hunter, Vibrational–translational/rotational and vibrational–vibrational processes in methane/inert-gas mixtures: optoacoustic phase measurements 74 (1983) 25
Aziz, R.A., W.J. Meath and A.R. Allnatt, On the Ne–Ne potential-energy curve and related properties 78 (1983) 295

Baas, F., see J.E.M. Haverkort 79 (1983) 105
Baer, T., see W.A. Brand 76 (1983) 111
Bagryansky, V.A., V.M. Zaskul'nikov and V.A. Tolkatchev, The kinetics of the retarded reaction of free radicals with oxygen in a methanol glass 78 (1983) 41
Baiardo, J., M. Vala and I. Trabjerg, The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. I. Single-crystal polarized absorption spectrum 79 (1983) 391
Baiardo, J. and M. Vala, The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. II. Calculation of spin–orbit coupling 79 (1983) 403
Baiardo, J., M. Vala and I. Trabjerg, The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. III. Single-crystal Zeeman spectroscopy 80 (1983) 305
Bailey, R.T., F.R. Cruickshank, D. Pugh, S. Guthrie, A. McLeod, W.S. Foulds, W.R. Lee and S. Venkatesh, The determination of thermal conductivity coefficients of liquids by a thermal lens technique 77 (1983) 243
Baker, J., EOM/propagator ionization potentials: extension of the excitation operator manifold 79 (1983) 117
Balint-Kurti, G.G. and M. Shapiro, Photofragmentation of triatomic molecules. Theory of angular and state distribution of product fragments, Chem. Phys. 61 (1981) 137. Erratum 72 (1982) 456
Baller, T., see G.N.A. van Veen 74 (1983) 261
Baller, T., see G.N.A. van Veen 80 (1983) 113
Bancroft, G.M., see D.J. Bristow 75 (1983) 263
Bancroft, G.M., D.J. Bristow and J.S. Tse, High-resolution HeI and HeII photoelectron spectra of the Zn 3d and Cd 4d orbitals in the zinc and cadmium dihalides: ligand field splittings and intensity variations 75 (1983) 277
Barańska, H., see W. Reimschüssel 72 (1982) 313
Barbé, R., see J.P. Astruc 75 (1983) 405
Barker, J.R., Monte Carlo calculations on unimolecular reactions, energy transfer, and IR-multiphoton decomposition 77 (1983) 301
Barone, V., F. Lelj, N. Russo, Y. Ellinger and R. Subra, Theoretical approach to fluorine substitution in X_2NO and X_2CN free radicals. Comparison between ab initio UHF and RHF + perturbation treatments 76 (1983) 385
Basilevsky, M.V., G.N. Gerasimov and S.I. Petrochenko, Calculations on the mechanism of ion polymerization in the formaldehyde crystal 72 (1982) 349
Bassi, D., A. Boschetti, G. Scoles, M. Scotoni and M. Zen, Infrared multiple photon excitation of sulfur hexafluoride in a molecular beam 71 (1982) 239
Bässler, H., see L. Sebastian 75 (1983) 103
Bässler, H., see R. Jankowiak 79 (1983) 57
Bässler, H., see G. Peter 80 (1983) 289
Basu, D., see S.S. Bhattacharyya 79 (1983) 129
Basu, S., K.A. McLauchlan and A.J.D. Ritchie, Flash photolysis electron spin resonance and CIDEP studies of radicals derived from nitrogen heterocyclics. I. The diazanaphthalenes 79 (1983) 95
Baumgärtel, H., see K. Rademann 80 (1983) 129
Bazhin, N.M., see V.I. Makarov 72 (1982) 213
Beenakker, J.J.M., see J.E.M. Beenakker 79 (1983) 105
Beijerinck, H.C.W., P.M.A. van der Kam and N.F. Verster, Glory undulations in the total cross section for Ar–Ar,Kr,Xe and Kr–Ar,Kr 72 (1982) 391
Beltran, D., see M. Drillon 79 (1983) 449
Benbow, R.L., see M.R. Thuler 71 (1982) 265
Benzel, M.A. and C.E. Dykstra, Conformational energetics in hydrogen-bonded dimers. The unobserved CO–HF complex 80 (1983) 273

Bergström, H., see V. Sundström 73 (1982) 439
Berman, M.R., J.W. Fleming, A.B. Harvey and M.C. Lin, Temperature dependence of the reactions of CH radicals with unsaturated hydrocarbons 73 (1982) 27
Bernstein, R.B., see S. Stolte 71 (1982) 353
Bernstein, R.B., see F.J. Aoiz 79 (1983) 321
Bernstein, R.B., see M.M. Oprysko 79 (1983) 341
Berréhar, J., C. Lapersonne-Meyer, M. Schott and M. le Postollec, Resonance Raman scattering and absorption spectroscopy of substituted polyenes 77 (1983) 11
Besnard, M., see J. Lascombe 72 (1982) 177
Bhar, G.C., see L.K. Samanta 79 (1983) 361
Bhattacharyya, S.N., see S. Ghosh 72 (1982) 161
Bhattacharyya, S.S. and D. Basu, Shape resonances and the photodissociation cross section of MgH near threshold 79 (1983) 129
Bigelow, R.W., Breakdown in the Koopmans' theorem interpretation of the outer valence-level photoemission spectra of selected organic molecules 80 (1983) 45
Billing, G.D., see L.L. Poulsen 73 (1982) 313
Billing, G.D., Semiclassical theory for atom–surface scattering: calculations on Ar + W(110) 74 (1983) 143
Billing, G.D., Semiclassical calculation of energy transfer in polyatomic molecules. VIII. Theory for atom + non-linear triatom 76 (1983) 315
Billing, G.D., Semiclassical calculation of energy transfer in polyatomic molecules. X. Energy transfer in Ar + SF_6 at 1 eV 79 (1983) 179
Billing, G.D. and D.C. Clary, Semiclassical calculation of energy transfer in polyatomic molecules. IX. Cross sections for M + $CO_2(000) \rightarrow$ M + $CO_2(nml)$ (M = He and Ar) 80 (1983) 213
Blackmore, R., see B. Shizgal 77 (1983) 417
Blomquist, J., U. Helgeson, B. Folkesson and R. Larsson, Studies of some iron dithiolate complexes by the ESCA, Mössbauer and extended Hückel methods 76 (1983) 71
Bly, S.H.P., see P. Arrowsmith 79 (1983) 31
Bock, C.W., M. Trachtman and P. George, An ab initio study of relationships between bond lengths and the harmonic and anharmonic cross-coupling constants involving the double bonds in hetero-atom substituted conjugated dienes 73 (1982) 179
Böhm, M.C., A crystal orbital investigation on the one-dimensional bis(glyoximato)pyrazine–iron system 76 (1983) 1
Boland, B.C., see J. Howard 77 (1983) 145
Bol'shakov, B.V., see V.L. Vyazovkin 75 (1983) 11
Bombach, R., J.-P. Stadelmann and J. Vogt, Unimolecular dissociations of excited $C_3H_6O^+$: a comparative photoelectron–photoion coincidence study of 1,2-epoxypropane and acetone 72 (1982) 259
Bombach, R., see J. Dannacher 75 (1983) 23
Bonazzola, L., N. Leray and Y. Ellinger, Ab initio calculations as first step towards the structure of free radicals. I. Geometries and energies of the ethyl analogs $NH_2CH_3^+$ and $CH_2NH_3^+$ 73 (1982) 145
Bonnett, J.D., see J.S. Geiger 74 (1983) 239
Bordé, Ch.J., see J. Bordé 71 (1982) 417
Bordé, J. and Ch.J. Bordé, Superfine and hyperfine structures in the ν_3 band of $^{32}SF_6$ 71 (1982) 417
Borsella, E., D. Masci, M. Capitelli and M. Dilonardo, Study of IR multiple-photon absorption (MPA) of CF_3Br 77 (1983) 401
Borshchevsky, A.Ya., see L.N. Sidorov 71 (1982) 145
Boschetti, A., see D. Bassi 71 (1982) 239

Botrel, A., F. Corre and A. le Beuze, Theoretical solvent effects on molecular structure and spectroscopic properties through the virtual-charge model. Application to the inverted solvatochromy of benzophenone $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ absorption bands 74 (1983) 383
Botschwina, P., J. Flesch and W. Meyer, Spectroscopic properties of the methyl radical calculated from UHF SCEP wavefunctions 74 (1983) 321
Botschwina, P., see D. Eisel 80 (1983) 329
Bougeard, D., see J. de Villepin 73 (1982) 291
Bouma, W.J., see M.J. Frisch 75 (1983) 323
Bounds, P.J., see I. Eisenstein 74 (1983) 307
Branca, M., A. Gamba, C. Oliva and M. Simonetta, Analysis of restricted rotation of the acetyl group in *m*- and *p*-nitroacetophenone anion radicals 75 (1983) 253
Brand, W.A., T. Baer and C.E. Klots, Kinetic energy release distribution in the fragmentation of energy-selected iodopropane ions 76 (1983) 111
Brieger, M., A. Renn, A. Sodeik and A. Hese, The dipole moment of ^{7}LiH and ^{7}LiD in the excited $A\,^1\Sigma^+$ state: a test of the Born–Oppenheimer approximation 75 (1983) 1
Brinkman, G.A., see E.Roduner 73 (1982) 117
Brion, C.E., see F. Carnovale 74 (1983) 253
Brion, C.E., see A. Minchinton 76 (1983) 89
Bristow, D.J., G.M. Bancroft and J.S. Tse, High-resolution HeI and HeII photoelectron spectra of the zinc and cadmium dihalide valence bands 75 (1983) 263
Bristow, D.J., see G.M. Bancroft 75 (1983) 277
Broyer, M., see S. Abed 74 (1983) 97
Brühlmann, U., see H.U. Zürcher 73 (1982) 403
Brutschy, B., see K. Rademann 80 (1983) 129
Buck, U., J. Kesper, H.H. Kuge and D. Otten, Relaxation and spectroscopy of CaCl in seeded supersonic beams 77 (1983) 201
Buckingham, M.R., see J.P. Martin 74 (1983) 15
Budenholzer, F.E. and C.-C. Lee, Classical differential cross sections and rotational energy transfer distributions for realistic ion–molecule potentials in the CPST limit 73 (1982) 323
Buenker, R.J., see B.A. Hess 71 (1982) 79
Buenker, R.J., see S.D. Peyerimhoff 72 (1982) 111
Buenker, R.J., see P.G. Burton 73 (1982) 83
Buenker, R.J., see R. Klotz 76 (1983) 367
Buff, R., see J. Dannacher 75 (1983) 23
Burshtein, A.I., see A.B. Doktorov 71 (1982) 1
Burshtein, A.I., see A.A. Kipriyanov 76 (1983) 149
Burshtein, A.I., see A.A. Kipriyanov 76 (1983) 163
Burton, P.G., S.D. Peyerimhoff and R.J. Buenker, Theoretical studies of the electronic spectrum of thioformaldehyde 73 (1982) 83
Burzyński, R. and T. Luty, Diamagnetic anisotropy of molecular complexes of 1,3,5-trinitrobenzene with anthracene and carbazole 72 (1982) 441
Butkovskaya, N.I., I.I. Morozov, V.L. Tal'rose and E.S. Vasiliev, Kinetic studies of the bromine–oxygen system: a new paramagnetic particle, BrO_2 79 (1983) 21
Butsky, V.D., see L.N. Sidorov 71 (1982) 145

Cacelli, I., R. Moccia and V. Carravetta, Electronic properties by Green's function calculations. Renormalized optical potential results: Ne, Ar, HF, H_2O, NH_3 71 (1982) 199
Califano, S., see R.G. Della Valle 74 (1983) 179
Campbell, E.J. and S.G. Kukolich, Electric dipole moments of $(HC^{15}N)_2$ and $HC^{15}NH^{35}Cl$ 76 (1983) 225
Capitelli, M., see E. Borsella 77 (1983) 401
Capitelli, M., C. Gorse, J. Wilhelm and R. Winkler, Collision dominated relaxation of electrons in a weakly ionized nitrogen plasma after abrupt change of the electric field 79 (1983) 1
Cardy, H., D. Liotard, A. Dargelos and E. Poquet, Ab initio study of the thermodynamic and kinetic stability of the ammonium radical 77 (1983) 287
Carlson, T.A., see P.R. Keller 74 (1983) 247
Carlson, T.A., see P.R. Keller 79 (1983) 269
Carlson, Th.A., see F.A. Grimm 80 (1983) 389
Carmeli, B., R. Tulman, A. Nitzan and M.H. Kalos, Random coupling models. IV. Numerical investigation of the dependence on the random coupling distribution and on the initial phases 72 (1982) 363
Carnovale, F. and C.E. Brion, Absolute dipole oscillator strengths for molecular and dissociative photoionization of hydrogen fluoride 74 (1983) 253
Carravetta, V., see I. Cacelli 71 (1982) 199
Carré M., see S. Abed 74 (1983) 97
Cartwright, D.J., see M.M. Maricq 75 (1983) 347
Casalegno, R., see R.J.D. Miller 72 (1982) 371
Castex, M.-C. see Th. Moeller 76 (1983) 295
Castleman Jr., A.W., see V. Hermann 72 (1982) 185
Casu, M., see A. Lai 71 (1982) 271
Cataliotti, R. and G. Paliani, Phonon spectra and structure of crystalline ethylene oxide and ethylene sulphide at 77 K 72 (1982) 293
Celli, V., see N.R. Hill 73 (1982) 363
Chakravorty, K.K., see S. Stolte 71 (1982) 353
Chalapati Rao, Y.V. and B.V. Mallu, Vibrational relaxation times in polyatomic gas mixtures: on the validity of the linear mixture rule 74 (1983) 43
Chang, C.C., see P.J. Kuntz 75 (1983) 79
Chapman, S., M. Dupuis and S. Green, Theoretical three-dimensional potential-energy surface for the reaction of Be with HF 78 (1983) 93
Chapuisat, X., see A. Nauts 76 (1983) 349
Charters, P.E., see P. Arrowsmith 79 (1983) 31
Châtelet, M., J. Kieffer and B. Oksengorn, Vibrational energy relaxation of highly compressed gaseous H_2 and N_2 79 (1983) 413
Chawla, G.K., see S.J. Silvers 80 (1983) 177
Chen, K.-M. and C.-C. Pei, Photodissociation kinematics. II. Laboratory angular distributions of a hydride model system and the kinematic isotope effect 76 (1983) 219
Chen (Dschen), T., F. Graf and Hs.H. Günthard, The ESR spectrum of the C_5F_5 radical 75 (1983) 165
Chenery, J.A., see J.P. Martin 74 (1983) 15
Chevrier, P., see P. Arrowsmith 79 (1983) 31
Chhor, K., see G. Lucazeau 76 (1983) 307
Choi, J.G. and G.J. Diebold, Microphone detection of pulsed atomic and molecular beams 73 (1982) 19
Chollet, P.-A. and J. Messier, Studies of oriented Langmuir–Blodgett multilayers by infrared linear dichroism 73 (1982) 235
Cirelli, G., T.-K. Ha, R. Meyer and Hs.H. Günthard, α-hydroxyalkyl radicals by photoreduction in aprotic solvents: ESR spectra, ab initio potential function, inversion–internal rotation dynamics and temperature dependence of coupling constants of 1-hydroxyethyl 72 (1982) 15

Clary, D.C., Exchange reactions of hydrogen halides with hydrogenic atoms 71 (1982) 117
Clary, D.C., New type of rotational basis function for quantum-mechanical molecular collision calculations 76 (1983) 331
Clary, D.C., see G.D. Billing 80 (1983) 213
Clouthier, D.J. and C.M.L. Kerr, Determination of the dipole moment of thioformaldehyde in the $\tilde{a}^3A_2$ excited state by laser phosphorescence excitation spectroscopy 80 (1983) 299
Clyne, M.A.A. and A. Hodgson, Kinetics and detection of F (^2P) atoms in a discharge flow system 79 (1983) 351
Cofino, W.P., G.Ph. Hoornweg, C. Gooijer, C. MacLean and N.H. Velthorst, Highly resolved optical spectra of *o*-durylene 72 (1982) 73
Collin, J.E., see P. Natalis 73 (1982) 191
Collins, M.A. and D.P. Craig, A model of localization, soliton propagation, and self-trapping in an electronically excited atomic lattice 75 (1983) 191
Colonna, F.P., see G. Distefano 72 (1982) 267
Colonna, F.P., see A. Modelli 77 (1983) 153
Colwell, S.M. and I.C. Percival, The semiclassical determination of potential surfaces from observed spectra. I 75 (1983) 215
Colwell, S.M. and I.C. Percival, The semiclassical determination of potential surfaces from observed spectra. II 75 (1983) 225
Comes, F.J., see K.-H. Stephan-Rossbach 80 (1983) 121
Consiglio, G., see G. Distefano 72 (1982) 267
Cook, J.P.D., see A. Minchinton 76 (1983) 89
Coronado, E., see M. Drillon 79 (1983) 449
Corre, F., see A. Botrel 74 (1983) 383
Corvaja, C., see G. Agostini 77 (1983) 233
Craig, D.P. and I.R. Elsum, Chiral discrimination in the liquid state: a hard-core model for the rôle of repulsive forces 73 (1982) 349
Craig, D.P., see M.A. Collins 75 (1983) 191
Criag, D.P., see K. Norris 79 (1983) 9
Creagh, A.L., see D.K. Evans 80 (1983) 379
Cramarossa, F., see S. de Benedictis 71 (1982) 247
Crisponi, G., see A. Lai 71 (1982) 271
Cruickshank, F.R., see R.T. Bailey 77 (1983) 243
Cureton, C.G., see P.C. Alford 76 (1983) 103

D'Agostino, R., see S. de Benedictis 71 (1982) 247
Dakhnovskii, Yu.I. and A.A. Ovchinnikov, Charge transfer in polar media. Transition-state entropy 80 (1983) 17
Dannacher, J., H.M. Rosenstock, R. Buff, A.C. Parr, R.L. Stockbauer, R. Bombach and J.-P. Stadelmann, Benchmark measurement of iodobenzene ion fragmentation rates 75 (1983) 23
Dargelos, A., see H. Cardy 77 (1983) 287
Daudey, J.-P., see S. Evangelisti 75 (1983) 91
Day, R.L. and L.C. Lee, Photoabsorption spectrum of radicals produced by a pulsed discharge of trace H_2O in Ar 75 (1983) 17
De Alti, G., P. Decleva and A. Lisini, MS Xα and LCAO Xα calculations of ionization potentials. A comparison with Koopmans' theorem and accurate calculations 76 (1983) 185
De Alti, G., P. Decleva and A. Lisini, Theoretical study of shake-up in the core photoelectron spectra of the alkali atoms 80 (1983) 229
Deb, B.M., see S.K. Ghosh 71 (1982) 295
De Benedictis, S., R. d'Agostino and F. Cramarossa, Spectroscopic analysis of the vibrational distributions in dissociative CO–He RF discharges 71 (1982) 247
Decleva, P., see G. de Alti 76 (1983) 185
Decleva, P., see G. de Alti 80 (1983) 229
Dedieu, A., see M.-M. Rohmer 77 (1983) 449
De Haas, M.P. and J.M. Warman, Photon-induced molecular charge separation studied by nano second time-resolved microwave conductivity 73 (1982) 35
Dehmer, J.L., see P.M. Dittman 78 (1983) 405
Della Valle, R.G., P.F. Fracassi, R. Righini and S. Califano, Anharmonic processes in molecular crystals. Calculation of the anharmonic shifts, bandwidths and energy decay processes in crystalline naphthalene 74 (1983) 179
Dellepiane, G., see P. Piaggio 77 (1983) 185
Demtröder, W., see D. Eisel 80 (1983) 329
De Rosny, G., see J. Perrin 73 (1982) 383
Desai, V.P., see E. König 80 (1983) 263
De Villepin, J., A. Novak and D. Bougeard, α- and β-phases of oxalic acid, $H_2C_2O_4$: vibrational spectra, normal-coordinate calculations, and intermolecular forces 73 (1982) 291
De Vries, A.E., see G.N.A. van Veen 74 (1983) 261
De Vries, A.E., see G.N.A. van Veen 80 (1983) 113
De Vries, M.S. and R.M. Martin, Vibrational effects with excitation transfer in metastable rare-gas–halide collisions 80 (1983) 157
Dexpert-Ghys, J., see P. Tola 78 (1983) 339
Dexpert-Ghys, J., see J. Goulon 78 (1983) 347
Dianoux, A.J., see G. Lucazeau 76 (1983) 307
Dick, B. and R.M. Hochstrasser, Resonant non-linear spectroscopy in strong fields 75 (1983) 133
Dick, B. and B. Nickel, Accessibility of the lowest quintet state of organic molecules through triplet–triplet annihilation; an INDO CI study 78 (1983) 1
Diebold, G.J., see J.G. Choi 73 (1982) 19
Diem, M., T.-L. Tso and E.K.C. Lee, Some observations on molecular complexes of carbon monoxide in argon and oxygen matrices 73 (1982) 283
Diercksen, G.H.F., M. Jaszuński and A.J. Sadlej, Near-degeneracy effects and efficiency of MBPT calculations of molecular properties. Polarizability curve of H_2 71 (1982) 105
Diercksen, G.H.F., V. Kellö, B.O. Roos and A.J. Sadlej, Perturbation theory of the electron correlation effect for atomic and molecular properties. VI. Complete active space (CAS) SCF and MBPT calculations of electric properties of the FH molecule 77 (1983) 93

Diercksen, G.H.F. and A.J. Sadlej, Finite-field many-body perturbation theory. VI. Multipole polarizabilities of beryllium. A comparative study 77 (1983) 429
Di Lauro, C. and F. Lattanzi, Fermi-coupled spherically adapted effective states in the collisionless multiphoton excitation of SF_6 71 (1982) 233
Di Lauro, C., F. Lattanzi and G. Sanna, Concurrence of the $n\nu_3$ and $(n-1)\nu_3+\nu_2+\nu_6$ vibrational ladders in the collisionless multiphoton excitation of $^{32}SF_6$ 73 (1982) 215
Dill, D., see P.M. Dittman 78 (1983) 405
Dilonardo, M., see E. Borsella 77 (1983) 401
Dissado, L.A., see R. Nigmatullin 79 (1983) 455
Distefano, G., M. Guerra, F.P. Colonna, D. Jones, G. Consiglio and D. Spinelli, Intense shake-up satellites in the XPS spectra of planar and sterically hindered N-piperidyl-nitrobenzenes and -nitrothiophens 72 (1982) 267
Distefano, G., see A. Modelli 73 (1982) 395
Distefano, G., see A. Modelli 77 (1983) 153
Dittmann, P.M., D. Dill and J.L. Dehmer, Valence-shell photoabsorption by CO_2 and its connections with electron–CO_2 scattering 78 (1983) 405
Doktorov, A.B., O.A. Anisimov, A.I. Burshtein and Yu.N. Molin, Theory of optically detected magnetic resonance spectra of radical pairs 71 (1982) 1
Doktorov, A.B., see A.A. Kipriyanov 76 (1983) 149
Doktorov, A.B., see A.A. Kipriyanov 76 (1983) 163
Dolg, M., see J. Flad 75 (1983) 331
Dorfmüller, Th., see M. Geilhaupt 76 (1983) 443
Dörr, F., see G.J. Woolfe 77 (1983) 213
Doyennette, L., see F. Al Adel 74 (1983) 413
Drevillon, B., see J. Perrin 73 (1982) 383
Drillon, M., E. Coronado, D. Beltran and R. Georges, Classical treatment of a Heisenberg linear chain with spin alternation; application to the MnNi (EDTA)·$6H_2O$ complex 79 (1983) 449
Drolshagen, G. and J.P. Toennies, Breathing-sphere quantum calculations of integral and differential cross sections for vibrational excitation in ion (atom)–diatom collisions 79 (1983) 159
Druzhinin, S.I. and B.M. Uzhinov, The mechanism of fluorescence quenching of aromatic compounds by acids: ZDO calculations 78 (1983) 29
Dubois, J.-E., see B. Ancian 74 (1983) 171
Dufayard, J. and O. Nedelec, Collision transfers between CdH A $^2\Pi$ $v'=0$ rotational states induced by He or Ar 71 (1982) 279
Dunbar, R.C., see N.B. Lev 80 (1983) 367
Dunmur, D.A. and R.W. Munn, The shape of the Lorentz cavity and the internal field in anisotropic fluids 76 (1983) 249
Duperrex, R., see J. Moser 79 (1983) 277
Dupuis, M., see S. Chapman 78 (1983) 93
Dykstra, C.E., see M.A. Benzel 80 (1983) 273

Easteal, A.J., P.V. Giaquinta, N.H. March and M.P. Tosi, Chemical effects in diffusion and structure of zinc chloride in aqueous solution 76 (1983) 125
Ebata, T., see M. Fujii 77 (1983) 191
Eberhardt, J.E., I.E. Hoare, D.A. Johnson, R.B. Knott, A.W. Pryor and A.B. Waugh, Multiphoton dissociation of some volatile uranyl complexes. I. The phenomena of reversible and permanent dissociation 72 (1982) 41
Eberhardt, J.E., R.B. Knott and A.W. Pryor, Multiphoton dissociation of some volatile uranyl complexes. II. Frequency and isotope effects 72 (1982) 51
Eberle, B., see H. Sontag 80 (1983) 279
Egdell, R.G., M. Hotokka, L. Laaksonen, P. Pyykkö and J.G. Snijders, Photoelectron spectra and their relativistic interpretation for gaseous bismuth trihalides 72 (1982) 237
Egelstaff, P.A. and J.H. Root, The temperature dependence of the structure of water 76 (1983) 405
Eisel, D., W. Demtröder, W. Müller and P. Botschwina, Autoionization spectra of Li_2 and the $X\,^2\Sigma_g^+$ ground state of Li_2^+: experimental and theoretical investigations 80 (1983) 329
Eisenstein, I., R.W. Munn and P.J. Bounds, Polarization energy of a localized charge in a molecular crystal. IV. Effect of polarizability changes 74 (1983) 307
Eisenstein, I. and R.W. Munn, Polarization energy of a localized charge in a molecular crystal. V. Effect of vacancies 77 (1983) 47
Eisenstein, I. and R.W. Munn, Polarization energy of a localized charge in a molecular crystal. VI. Effect of excitons 79 (1983) 189
Elbert, S.T., see K. Ruedenberg 71 (1982) 41
Elbert, S.T., see K. Ruedenberg 71 (1982) 65
Ellenbroek, T. and J.P. Toennies, A semiclassical model for the vibrational excitation of spherical-top molecules in collisions with ions 71 (1982) 309
Ellinger, Y., see L. Bonazzola 73 (1982) 145
Ellinger, Y., see V. Barone 76 (1983) 385
Elsum, I.R., see D.P. Craig 73 (1982) 349
Enkelmann, V., see D. Siegel 72 (1982) 201
Enkelmann, V., see W. Höptner 73 (1982) 253
Ern, V., see A. Fort 80 (1983) 205
Ernst, W.E. and J.O. Schröder, The $B\,^2\Sigma^+ - X\,^2\Sigma^+$ system of SrF: precise spectroscopic contants from a combined fit of microwave and sub-Doppler optical spectra 78 (1983) 363
Esherick, P., A.J. Grimley and A. Owyoung, Stimulated Raman investigation of CO_2-laser-excited SF_6 73 (1982) 271
Evangelisti, S., J.-P. Daudey and J.-P. Malrieu, Convergence of an improved CIPSI algorithm 75 (1983) 91
Evans, D.J. and G.P. Morriss, Isothermal–isobaric molecular dynamics 77 (1983) 63
Evans, D.K., R.D. McAlpine, H.M. Adams and A.L. Creagh, Intensity dependence of CO_2-laser-induced multiphoton absorption and decomposition of monomethylamine 80 (1983) 379
Evans, M.W., see M. Ferrario 72 (1982) 141
Evans, M.W., see M. Ferrario 72 (1982) 147
Even, U., see G. Smulevich 73 (1982) 1
Even, U., see G. Smulevich 76 (1983) 147

Farantos, S.C., Evaluation of an upper bound of the maximal Lyapunov characteristic number by Monte Carlo integration in the chaotic regions of phase space 71 (1982) 157
Fayer, M.D., see R.J.D. Miller 72 (1982) 371
Felder, P. and Hs.H. Günthard, Conformational interconversions in supersonic jets: matrix IR spectroscopy and model calculations 71 (1982) 9
Ferguson, J. and F. Herren, A model for the interpretation of the electronic spectra of the complex ions $M(bpy)_3^{2+}$ (M = Fe, Ru, Os) in D_3 and C_2 sites 76 (1983) 45
Ferrario, M. and M.W. Evans, Molecular dynamics computer simulation of liquid dichloromethane. I. Equilibrium properties 72 (1982) 141
Ferrario, M. and M.W. Evans, Computer simulation of dichloromethane. II. Molecular dynamics 72 (1982) 147
Ficocelli Varracchio, E., Quantum-mechanical rearrangement processes: off-shell vibro-rotational sudden approximation to the dynamics 74 (1983) 153
Fillaux, F., Theoretical model for calculations of infrared and Raman band profiles of strong hydrogen bonds in ordered media 74 (1983) 395
Fillaux, F., Calculations of infrared and Raman band profiles of strong hydrogen bonds. OH stretching bands and proton dynamics in crystalline potassium hydrogen carbonate 74 (1983) 405
Fincham, D. and D.M. Heyes, Comparisons between experimental argon and Lennard-Jones 12:6 shear viscosities 78 (1983) 425
Fink, E.H., see J. Wildt 80 (1983) 167
Fischer, G., R.E. Miller and R.O. Watts, Vibrational predissociation of van der Waals clusters of ethylene 80 (1983) 147
Fish, J.L., see D.D. Konowalow 77 (1983) 435
Flad, J., G. Igel, M. Dolg, H. Stoll and H. Preuss, A combination of pseudopotentials and density functionals: results for Li_n^{m+}, Na_n^{m+} and K_n^{m+} clusters ($n \leqslant 4$; $m = 0,1$) 75 (1983) 331
Flament, J.P., see D. Solgadi 79 (1983) 225
Fleming, J.W., see M.R. Berman 73 (1982) 27
Flesch, J., see P. Botschwina 74 (1983) 321
Folkesson, B., see J. Blomquist 76 (1983) 71
Forstmann, F., see C.M. Weinert 80 (1983) 95
Fort, A., V. Ern and V.M. Kenkre, Theory of coherence effects in time-dependent delayed fluorescence. II. Application to two- and three-dimensional crystals 80 (1983) 205
Foti, G., see O. Puglisi 75 (1983) 417
Foulds, W.S., see R.T. Bailey 77 (1983) 243
Fracassi, P.F., see R.G. Della Valle 74 (1983) 179
Freed, K.F., see A.A. Villaeys 72 (1982) 1
Frisch, M.J., K. Raghavachari, J.A. Pople, W.J. Bouma and L. Radom, Unusual low-energy isomers for simple radical cations 75 (1983) 323
Fröhling, W., C.J. Winscom and K. Möbius, Measurement of the ^{14}N nuclear quadrupole couplings in the lowest ($n\pi^*$) excited triplet state of pyrazine by ODMR 75 (1983) 389
Fujii, M., T. Ebata, N. Mikami and M. Ito, Electronic spectra of jet-cooled azulene 77 (1983) 191
Fuss, W., Comment on collisionless vibrational relaxation 76 (1983) 343

Gaillard, M.L., see S. Abed 74 (1983) 97
Gamba, A., see M. Branca 75 (1983) 253
Gardiner, D.J., see W.F. Pacynko 78 (1983) 319
Gauthier, M., see K.O. Kutschke 78 (1983) 323
Gaw, J.F., see Y. Osamura 72 (1982) 131
Geiger, J.S., D.R. Smith and J.D. Bonnett, Detection of transient laser magnetic resonance signals in pulsed CO_2 laser irradiation of SF_6/H_2O and SF_6/NO mixtures 74 (1983) 239
Geiger, L.C. and G.C. Schatz, A new approach to the determination of good action–angle variables for coupled oscillator systems 79 (1983) 431
Geilhaupt, M. and Th. Dorfmüller, Solvent effects on the potential energy surfaces of molecular iodine: a spectroscopic study 76 (1983) 443
Gentry, W.R., see R.T. Skodje 74 (1983) 347
George, P., see C.W. Bock 73 (1982) 179
Georges, R., see M. Drillon 79 (1983) 449
Gerasimov, G.N., see M.V. Basilevsky 72 (1982) 349
Ghosh, D.K., see L.K. Samanta 79 (1983) 361
Ghosh, S., D. Mukherjee and S.N. Bhattacharyya, A spin-adapted linear response theory in a coupled-cluster framework direct calculation of spin-allowed and spin-forbidden transition energies 72 (1982) 161
Ghosh, S.K. and B.M. Deb, Dynamic polarizability of many-electron systems with a time-dependent density-functional theory 71 (1982) 295
Giacometti, G., see G. Agostini 77 (1983) 233
Gianturco, F.A., U.T. Lamanna and G. Petrella, He–HF vibrational inelasticity at low and intermediate energies from quantum collision theory 78 (1983) 81
Giaquinta, P.V., see A.J. Easteal 76 (1983) 125
Giese, C.F., see R.T. Skodje 74 (1983) 347
Gilbert, M.M., see K. Ruedenberg 71 (1982) 41
Gilbert, M.M., see K. Ruedenberg 71 (1982) 51
Gilbert, M.M., see K. Ruedenberg 71 (1982) 65
Gilbert, R.G., see M.J. Riley 72 (1982) 83
Gilchrist, J. and H. Godfrin, Secondary amines: a low-temperature dielectric relaxation study 79 (1983) 307
Gilchrist, J., Primary amines: a low-temperature dielectric relaxation study 80 (1983) 63
Gillbro, T., see V. Sundström 73 (1982) 439
Gillies, R. and A.M. Ponte Goncalves, Driven-echo and rotary-echo measurements of the spin coherence in triplet-state benzophenone 78 (1983) 49
Girerd, J.J. and J.P. Launay, A model for two-electron four-center mixed valence systems. Application to $[W_4O_8Cl_8(H_2O)_4]^{2-}$ 74 (1983) 217
Godfrin, H., see J. Gilchrist 79 (1983) 307
Golab, J.T., D.L. Yeager and P. Jørgensen, Proper characterization of MC SCF stationary points 78 (1983) 175
Gooijer, C., see W.P. Cofino 72 (1982) 73
Gorse, C., see M. Capitelli 79 (1983) 1
Goulon, J., see P. Tola 78 (1983) 339
Goulon, J., P. Tola, M. Lemonnier and J. Dexpert-Ghys, On a site-selective EXAFS experiment using optical emission 78 (1983) 347
Goursaud, S., see G. Parlant 75 (1983) 175
Graf, F., see T. Chen 75 (1983) 165
Graham, D.J. and T.-S. Lin, High-resolution absorption spectra of diphenylmethylenes 73 (1982) 411
Grattan, K.T.V., see L. Hellner 80 (1983) 345

Gray, P., see K. Norris 79 (1983) 9
Gray, S.K., Classical aspects of the laser excitation of a Morse oscillator 75 (1983) 67
Green, R.S., see U.P. Agarwal 74 (1983) 35
Green, S., see S. Chapman 78 (1983) 93
Gregory, E.A., see M.M. Maricq 75 (1983) 347
Grimley, A.J., see P. Esherick 73 (1982) 271
Grimm, F.A., see P.R. Keller 74 (1983) 247
Grimm, F.A., see P.R. Keller 79 (1983) 269
Grimm, F.A., and Th.A. Carlson, Angular distribution for the major photoelectron bands of nitrogen below 45 eV binding energy 80 (1983) 389
Grimm, M., see H.J. Werner 73 (1982) 169
Grinter, R., see C.M. Weinert 80 (1983) 95
Gropen, O., see J. Müller 75 (1983) 395
Gropen, O., see L.G.M. Pettersson 80 (1983) 7
Guerra, M., see G. Distefano 72 (1982) 267
Günthard, Hs.H., see P. Felder 71 (1982) 9
Günthard, Hs.H., see G. Cirelli 72 (1982) 15
Günthard, Hs.H., see F.J. Rákóczi 74 (1983) 273
Günthard, Hs.H., see T. Chen 75 (1983) 165
Gupta, S., J.M. Haile and W.A. Steele, Use of computer simulation to determine the triplet distribution function in dense fluids 72 (1982) 425
Gürtler, P., see Th. Moeller 76 (1983) 295
Guthrie, S., see R.T. Bailey 77 (1983) 243
Gutsev, G.L. and A.P. Klyagina, The electronic structure of chalcogen hexahalogenides 75 (1983) 243

Ha, T.-K., see G. Cirelli 72 (1982) 15
Ha, T.-K., see F.J. Rákóczi 74 (1983) 273
Haaks, D., see Th. Moeller 76 (1983) 295
Habitz, P., see P. Archirel 78 (1983) 213
Hackett, P.A., see D.M. Rayner 77 (1983) 349
Hackett, P.A., see K.O. Kutschke 78 (1983) 323
Haile, J.M., see S. Gupta 72 (1982) 425
Haley, L.V. and J.A. Koningstein, Raman spectroscopy from a picosecond-lived excited state of methyl orange 73 (1982) 263
Haley, L.V. and J.A. Koningstein, Space- and time-resolved resonance-enhanced vibrational Raman spectroscopy from a femtosecond-lived singlet excited state of β-carotene 77 (1983) 1
Haller, M., see N.R. Hill 73 (1982) 363
Hamada, Y., see K. Ichikawa 72 (1982) 301
Hanazaki, I., see R. Nakagaki 72 (1982) 93
Handy, N.C., see P.J. Knowles 72 (1982) 337
Hanson, D.M., see J.S. Patel 72 (1982) 35
Hanuza, J., see Z. Mazurak 79 (1983) 255
Harvey, A.B., see M.R. Berman 73 (1982) 27
Hashimoto, K., A theoretical estimate for quasihomopolar singlet levels in long polyenes with a spin model hamiltonian 80 (1983) 253
Häusler, D. and R. Schinke, Theoretical investigation of rotational rainbows in $K + N_2$ and $K + CO$ collisions 79 (1983) 147
Haverkort, J.E.M., F. Baas and J.J.M. Beenakker, Measurements of depolarization ratios of gaseous linear chain molecules: a test of the principle of the additivity of bond polarizabilities 79 (1983) 105
Haynes, J.S., A.R. Hume, J.R. Sams and R.C. Thompson, Mössbauer spectroscopic study of the electronic and magnetic properties of iron(II) para-toluenesulphonate 78 (1983) 127
Helgeson, U., see J. Blomquist 76 (1983) 71
Hellner, L., K.T.V. Grattan and M.H.R. Hutchinson, Determination of rate constants for some reactions of CBr radicals by VUV laser flash photolysis 80 (1983) 345
Helman, A.B., On the theory of adiabatic electron-transfer reactions in polar solvents 79 (1983) 235
Helvajian, H., see H.H. Nelson 73 (1982) 431
Henry, L., see F. Al Adel 74 (1983) 413
Herman, I.P., Two-frequency CO_2 laser multiple-photon dissociation and dynamics of excited state absorption in CDF_3 75 (1983) 121
Hermann, V., B.D. Kay and A.W. Castleman Jr., Evidence for the existence of structures in gas-phase homomolecular clusters of water 72 (1982) 185
Hermanowicz, K., see Z. Mazurak 79 (1983) 255
Herren, F., see J. Ferguson 76 (1983) 45
Herscovitz, O., E. Tzidoni and I. Oref, Intermolecular energy-transfer probabilities of strong colliders 71 (1982) 221
Hese, A., see M. Brieger 75 (1983) 1
Hess, B.A., R.J. Buenker, C.M. Marian and S.D. Peyerimhoff, Ab initio calculation of the zero-field splittings of the $X\,^3\Sigma_g^-$ and $B\,^3\Pi_{g,i}$ states of the S_2 molecule 71 (1982) 79
Hess, B.A., see R. Klotz 76 (1983) 367
Hesselink, W.H., see J.B.W. Morsink 71 (1982) 289
Heyes, D.M., see D. Fincham 78 (1983) 425
Higelin, D. and H. Sixl, Spectroscopic studies of the photochromism of N-salicylideneaniline mixed crystals and glasses 77 (1983) 391

Higo, M., S. Kamata and T. Ogawa, Electron impact dissociation of molecular hydrogen and deuterium: isotope effect on the emission cross section of H^* and D^* (n = 3,4,5) 73 (1982) 99
Hill, N.R., M. Haller and V. Celli, Van der Waals forces and molecular diffraction from metal surfaces, with application to Ag(111) 73 (1982) 363
Hino, S., T. Veszprémi, K. Ohno, H. Inokuchi and K. Seki, Absorption spectra of volatile aromatic hydrocarbon films in the vacuum ultraviolet region 71 (1982) 135
Hirao, K. and S. Yamabe, Theoretical study on the structure and stability of hydrogen-ion clusters H_n^+ and H_n^- (n = 3,5,7,9,11,13) 80 (1983) 237
Hoare, I.E., see J.E. Eberhardt 72 (1982) 41
Hochstrasser, R.M., see B. Dick 75 (1983) 133
Hodgson, A., see M.A.A. Clyne 79 (1983) 351
Hoeft, J., see Ch. Ryzlewicz 71 (1982) 389
Hoffman III, W.F. and J.S. Shirk, Infrared laser photoisomerization of 2-fluoroethanol in argon 78 (1983) 331
Hoffmeister, M., L. Potthast and H.J. Loesch, State-selected molecular-beam reaction dynamics of K with HF (v = 1, j = 5,6 and 7) 78 (1983) 369
Höller, R., see Th. Weller 72 (1982) 155
Holmlid, L., see K. Rynefors 74 (1983) 446
Holten, D., see D. Kim 75 (1983) 305
Hoornweg, G.Ph., see W.P. Cofino 72 (1982) 73
Höptner, W., M. Mehring, J.U. von Schütz, H.C. Wolf, B.S. Morra, V. Enkelmann and G. Wegner, Magnetic resonance experiments on the radical cation salt (fluoranthenyl)$_2^+PF_6^-$. Correlation of proton-NMR, fluorine-NMR and ESR 73 (1982) 253
Hormes, J. and J. Schiller, Jahn–Teller splitting of the 3s → 3p transition of sodium isolated in a xenon matrix 74 (1983) 433
Hotokka, M., see A. Viste 72 (1982) 225
Hotokka, M., see R.G. Egdell 72 (1982) 237
Howard, J., B.C. Boland and J. Tomkinson, Intensities in inelastic neutron scattering spectra: a test of recent theory 77 (1983) 145
Huber, J.R., see H.U. Zürcher 73 (1982) 403
Huc, J., see J. Perrin 73 (1982) 383
Hulsman, H., see P. Willems 71 (1982) 27
Hume, A.R., see J.S. Haynes 78 (1983) 127
Hunter, T.F., see E. Avramides 74 (1983) 25
Hurych, Z., see M.R. Thuler 71 (1982) 265
Hutchinson, M.H.R., see L. Hellner 80 (1983) 345

Ichikawa, K., Y. Hamada, Y. Sugawara, M. Tsuboi, S. Kato and K. Morokuma, Ab initio study on cyanamide and isocyanamide 72 (1982) 301
Igel, G., see J. Flad 75 (1983) 331
Inokuchi, H., see S. Hino 71 (1982) 135
Inokuchi, H., see N. Sato 76 (1983) 79
Islampour, R. and M. Kasha, Molecular translational–rovibronic hamiltonian. I. Non-linear molecules 74 (1983) 67
Islampour, R. and M. Kasha, Molecular translational–rovibronic hamiltonian. II. Linear molecules 75 (1983) 157
Ito, H., see Y. Ozaki 80 (1983) 85
Ito, M., see M. Fujii 77 (1983) 191
Ito, Y., see I. Tokue 79 (1983) 383

Jacobs, J.W.M., see W. Ravenek 78 (1983) 391
Jacobsen, F.M., see O.E. Mogensen 73 (1982) 223
Jakubetz, W., The orientation-averaged rotation-decoupled vibration model for product state distributions in light+heavy–heavy reactions 75 (1983) 45
Jalmukhambetov, A.U. and I.S. Osad'ko, Dependence of photochemical and photophysical hole burning on laser intensity 77 (1983) 247
Jankowiak, R. and H. Bässler, Dispersive singlet exciton motion in an organic glass 79 (1983) 57
Jarzeba, W., see J. Najbar 79 (1983) 245
Jaszuński, M., see G.H.G. Diercksen 71 (1982) 105
Jeżowska-Trzebiatowska, B., see Z. Mazurak 79 (1983) 255
Johansen, H. and S. Rettrup, Limited configuration interaction calculation of the optical spectrum for the permanganate ion 74 (1983) 77
Johnson, D.A., see J.E. Eberghardt 72 (1982) 41
Jones, D., see G. Distefano 72 (1982) 267
Jones, D., see A. Modelli 73 (1982) 395
Jones, D., see A. Modelli 77 (1983) 153
Jordan, B., see Th. Moeller 76 (1983) 295
Jørgensen, P., see T.L. Golab 78 (1983) 175
Jortner, J., see M.L. Sage 72 (1982) 249
Jortner, J., see G. Smulevich 73 (1982) 1
Jortner, J., see G. Smulevich 76 (1983) 147
Jung, Ch., A. Lau, H.-J. Weigmann, W. Werncke and M. Pfeiffer, Interpretation of resonance CARS and Shpolskii spectra with calculated molecular geometries, vibrational frequencies and relative intensities: chrysene in its lowest excited singlet and triplet state 72 (1982) 327
Jungen, M., see K. Kaufmann 79 (1983) 111

Kalos, M.H., see B. Carmeli 72 (1982) 363
Kamata, S., see M. Higo 73 (1982) 99
Kanellakopulos, B., see E. König 80 (1983) 263
Karlsson, L., see I. Reineck 78 (1983) 311
Karpfen, A., Ab initio studies on hydrogen-bonded chains. III. The linear, infinite chain of hydrogen cyanide molecules 79 (1983) 211
Kasatani, K., see M. Kawasaki 73 (1982) 377
Kasatani, K., see M. Kawasaki 74 (1983) 83
Kasatani, K., see M. Kawasaki 78 (1983) 65
Kasha, M., see R. Islampour 74 (1983) 67
Kasha, M., see R. Islampour 75 (1983) 157
Kato, S., see K. Ichikawa 72 (1982) 301
Kaufmann, K., M. Jungen and V. Staemmler, Can the H_5 molecule be observed? 79 (1983) 111
Kawasaki, M., K. Kasatani, H. Sato, H. Shinohara and N. Nishi, Photodissociation of molecular beams of SO_2 at 192 nm 73 (1982) 377
Kawasaki, M., K. Kasatani, Y. Ogawa and H. Sato, Spectra and emission lifetimes of $H_2CS(\tilde{A}\,^1A_2)$ 74 (1983) 83
Kawasaki, M., K. Kasatani, H. Sato, H. Shinohara and N. Nishi, Photodissociation of molecular beams of N_2O_4 78 (1983) 65
Kay, B.D., see V. Hermann 72 (1982) 185
Keller, P.R., J.W. Taylor, F.A. Grimm, P. Senn, T.A. Carlson and M.O. Krause, Angle-resolved photoelectron measurements on the 2p orbitals of Si in SiF_4 and $Si(CH_3)_4$ in the gas phase 74 (1983) 247
Keller, P.R., J.W. Taylor, T.A. Carlson and F.A. Grimm, Angle-resolved photoelectron spectroscopy of the chloro-substitute methanes 79 (1983) 269
Kellö, V., see G.H.F. Diercksen 77 (1983) 93
Kenkre, V.M., see A. Fort 80 (1983) 205
Kerr, C.M.L., see D.J. Clouthier 80 (1983) 299
Kesper, J., see U. Buck 77 (1983) 201
Khanra, B.C. and S.K. Saha, An extended Hückel study of hydrogen and oxygen chemisorption on Ru(001) surface 76 (1983) 255
Khromov, I.E., see V.N. Sazonov 76 (1983) 25
Khumalo, F.S., see M. Piacentini 72 (1982) 61
Kieffer, J., see M. Châtelet 79 (1983) 413
Kim, D., C. Kirmaier and D. Holten, Nickel porphyrin photophysics and photochemistry. A picosecond investigation of ligand binding and release in the excited state 75 (1983) 305
Kimel, S., see D.M. Rayner 77 (1983) 349
Kimura, K., see S. Tomoda 74 (1983) 113
Kimura, K., see S. Tomoda 74 (1983) 121
Kipriyanov, A.A., A.B. Doktorov and A.I. Burshtein, Binary theory of dephasing in liquid solutions. I. The non-markovian theory of encounters 76 (1983) 149
Kipriyanov, A.A., A.B. Doktorov and A.I. Burshtein, Binary theory of dephasing in liquid solutions. II. Motion-transformed isotropic Raman spectra 76 (1983) 163
Kirmaier, C., see D. Kim 75 (1983) 305
Klapstein, D., J.P. Maier, L. Misev and W. Zambach, Emission and laser excitation spectra of rotationally cooled cations in the gas phase: $\tilde{A}\,^2\Pi \leftrightarrow \tilde{X}\,^2\Pi$ band system of $H(C{\equiv}C)_2X^+$, X = Cl, Br 72 (1982) 101
Klapstein, D., see S. Leutwyler 74 (1983) 441

Klapstein, D., J.P. Maier and W. Zambach, Emission spectra of rotationally cooled dihaloacetylene cations in the gas phase: $\tilde{A}\,^2\Pi_{\Omega,g}$ $\tilde{X}\,^2\Pi_{\Omega,u}$ band systems 77 (1983) 463
Klapstein, D., see S. Leutwyler 78 (1983) 151
Klapstein, D., R. Kuhn, S. Leutwyler and J.P. Maier, Emission spectra of supersonically cooled dimethyldiacetylene cations 78 (1983) 167
Klemp, D. and B. Nickel, Phosphorescence and E-type delayed fluorescence from azulene in phenazine host crystals 78 (1983) 17
Klomp, U.C. and J. Los, State-to-state total cross sections for ion-pair formation 71 (1982) 443
Klots, C.E., see W.A. Brand 76 (1983) 111
Klotz, R., C.M. Marian, S.D. Peyerimhoff, B.A. Hess and R.J. Buenker, Study of the dependence of spin–orbit matrix elements on AO basis set composition for inner and valence shells: results for the multiplet splitting of $X\,^3\Sigma^-$ and $C\,^3\Pi$ of SO and $X\,^2\Pi$ in SO^+ 76 (1983) 367
Klyagina, A.P., see G.L. Gutsev 75 (1983) 243
Knapp, E.W., see H.W. Krüger 74 (1983) 205
Knott, R.B., see J.E. Eberhardt 72 (1982) 41
Knott, R.B., see J.E. Eberhardt 72 (1982) 51
Knowles, P.J., G.J. Sexton and N.C. Handy, Studies using the CASSCF wavefunction 72 (1982) 337
Köhler, F.H., see E. König 80 (1983) 263
Köhler, H.J., see Th. Weller 72 (1982) 155
Kolb, D.M., see C.M. Weinert 80 (1983) 95
Kołodziej, H.A. and S. Sorriso, Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. I. Ferroelectric behaviour 77 (1983) 341
Kołodziej, H.A. and S. Sorriso, Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. II. Isotopic effect 78 (1983) 75
Komorowski, L., Fractionally charged ions in crystal lattices of organic ion-radical salts 76 (1983) 31
Kondow, T., see T. Nagata 72 (1982) 281
Kondow, T., see Y. Ozaki 77 (1983) 223
Kondow, T., see Y. Ozaki 80 (1983) 73
Kondow, T., see Y. Ozaki 80 (1983) 85
König, E., V.P. Desai, B. Kanellakopulos and F.H. Köhler, Magnetic susceptibility of 1,1′,2,2-tetramethylcabaltocene and 1,1′-diethylcobaltocene: evidence for the dynamic Jahn–Teller effect 80 (1983) 263
Koningstein, J.A., see L.V. Haley 73 (1982) 263
Koningstein, J.A., see L.V. Haley 77 (1983) 1
Konowalow, D.D. and J.L. Fish, Long-range interactions of Li(n = 2) states with each other and the long-range interaction of Li($2s\,^2S$) with Li($3s\,^2S$) 77 (1983) 435
Kopelman, R., see P. Argyrakis 78 (1983) 251
Köppel, H., Ultrafast non-radiative decay via conical intersections of molecular potential-energy surfaces: $C_2H_4^+$ 77 (1983) 359
Kotomin, E. and V. Kuzovkov, Some problems of recombination kinetics. I 76 (1983) 479
Koutecký, J., see G. Pacchioni 71 (1982) 181
Kowalewski, J., see A. Laaksonen 80 (1983) 221
Kratky, K.W., see W. Schreiner 80 (1983) 245
Krause, M.O., see P.R. Keller 74 (1983) 247
Krauss, R., W. Schrof, H.C. Wolf and D. Schmid, The motion of triplet excitons in β-phase crystals of 9,10-dichloroanthracene 73 (1982) 55
Krüger, H.W., M.E. Michel-Beyerle and E.W. Knapp, Electron hopping and magnetic field dependent spin dynamics of radical ions in solution 74 (1983) 205

Kuball, H.-G., see A. Schönhofer 76 (1983) 453
Kubodera, H., see K. Ohta 76 (1983) 271
Kuchitsu, K., see T. Nagata 72 (1982) 281
Kuchitsu, K., see Y. Ozaki 77 (1983) 223
Kuchitsu, K., see Y. Ozaki 80 (1983) 73
Kuchitsu, K., see Y. Ozaki 80 (1983) 85
Kuge, H.H., see U. Buck 77 (1983) 201
Kuhn, R., see D. Klapstein 78 (1983) 167
Kukolich, S.G., see E.J. Campbell 76 (1983) 225
Kuntz, P.J. and C.C. Chang, Semi-empirical corrections to the mixing coefficients for the diatomics-in-molecules method 75 (1983) 79
Kurzyński, M., see M. Pyda 79 (1983) 219
Kutschke, K.O., M. Gauthier and P.A. Hackett, Separation of deuterium by IR multiphoton decomposition of chlorodifluoromethane. IR multiphoton absorption by and decomposition of a CF_2DCl/CF_2HCl mixture 78 (1983) 323
Kuzovkov, V., see E. Kotomin 76 (1983) 479

Laaksonen, A., J. Kowalewski and V.R. Saunders, Finite perturbation MCSCF and CI calculations of nuclear spin–spin coupling constants for some molecules with multiple bonds 80 (1983) 221
Laaksonen, L., see A. Viste 72 (1982) 225
Laaksonen, L., see R.G. Egdell 72 (1982) 237
Łabudzinska, A., see W. Reimschüssel 72 (1982) 313
Lacey, A.R., see M.J. Riley 72 (1982) 83
Lagrèze, A., see J.P. Astruc 75 (1983) 405
Lahmani, F., see D. Solgadi 79 (1983) 225
Lai, A., M. Monduzzi, G. Saba, M. Casu and G. Crisponi, C-13 magnetic relaxation rates and H-1 and C-13 paramagnetic shifts of Ni(II) complex of dopamine 71 (1982) 271
Lamanna, U.T., see F.A. Gianturco 78 (1983) 81
Lampert, R.A., see P.C. Alford 76 (1983) 103
Lankhorst, D., J. Schriever and J.C. Leyte, An NMR relaxation study of hydrogen exchange and its deuterium isotope effects in aqueous carboxylic acid solutions 77 (1983) 319
Lapersonne-Meyer, C., see J. Berréhar 77 (1983) 11
Lardeux, C., see D. Solgadi 79 (1983) 225
Larsson, M. and P.E.M. Siegbahn, The radiative lifetime of the $A\,^1\Pi$ state of CH^+ calculated from long CAS SCF expansions 76 (1983) 175
Larsson, R., see J. Blomquist 76 (1983) 71
Larzillière, M., see S. Abed 74 (1983) 97
Lascombe, J., M. Besnard and P. Maraval, A new extended diffusion model for rotational motion of symmetric-top molecules in the liquid phase 72 (1982) 177
Lattanzi, F., see C. di Lauro 71 (1982) 233
Lattanzi, F., see C. di Lauro 73 (1982) 215
Lau, A., see Ch. Jung 72 (1982) 327
Launay, J.P., see J.J. Girerd 74 (1983) 217
Lavrik, N.L., see V.I. Makarov 72 (1982) 213
Le Beuze, A., see A. Botrel 74 (1983) 383
Le Calve, J., see Th. Moeller 76 (1983) 295
Ledoux, I. and J. Zyss, Influence of the molecular environment in solution measurements of the second-order optical susceptibility for urea and derivatives 73 (1982) 203
Lee, A.G., see S.R. Meech 80 (1983) 317
Lee, C.-C., see F.E. Budenholzer 73 (1982) 323
Lee, E.K.C., see M. Diem 73 (1982) 283
Lee, L.C., see R.L. Day 75 (1983) 17
Lee, W.R., see R.T. Bailey 77 (1983) 243
Legon, A.C. and L.C. Willoughby, The rotational spectrum and molecular properties of a hydrogen-bonded dimer of phosphine and hydrogen fluoride 74 (1983) 127
Lelj, F., see V. Barone 76 (1983) 385
Lemonnier, M., see P. Tola 78 (1983) 339
Lemonnier, M., see J. Goulon 78 (1983) 347
Le Postollec, M., see J. Berréhar 77 (1983) 11
Leray, N., see L. Bonazzola 73 (1982) 145
Lersch, W. and M.E. Michel-Beyerle, Magnetic field effects on the recombination of radical ions in reaction centers of photosynthetic bacteria 78 (1983) 115
Leutwyler, S., D. Klapstein and J.P. Maier, Anomalous rotational distributions in electronic emission of supersonically cooled H_2O^+ ($\tilde{A}\,^2A_1 \rightarrow \tilde{X}\,^2B_1$) 74 (1983) 441
Leutwyler, S., D. Klapstein and J.P. Maier, Emission spectra of supersonically cooled methyldiacetylene cations 78 (1983) 151

Leutwyler, S., see D. Klapstein 78 (1983) 167
Lev, N.B. and R.C. Dunbar, Infrared-enhanced multiphoton dissociation of iodobenzene cations 80 (1983) 367
Leveque, G., see M. Piacentini 72 (1982) 61
Leyte, J.C., see D. Lankhorst 77 (1983) 319
Liegener, C.-M., Double-ionization Auger satellites obtained by the Green's function method 76 (1983) 385
Likhansky, V.V. and G.A. Solodovnikov, Generalized Landau–Zener formula for non-adiabatic transitions between degenerate states 77 (1983) 409
Lin, M.C., see M.R. Berman 73 (1982) 27
Lin, T.-S., see D.J. Graham 73 (1982) 411
Liotard, D., see H. Cardy 77 (1983) 287
Lischka, H., see Th. Weller 72 (1982) 155
Lisini, A., see G. de Alti 76 (1983) 185
Lisini, A., see G. de Alti 80 (1983) 229
Lloret, A., see J. Perrin 73 (1982) 383
Lodin, P., see I. Reineck 78 (1983) 311
Loesch, H.J., see M. Hoffmeister 78 (1983) 369
Longton, L., see P. Natalis 73 (1982) 191
Los, J., see U.C. Klomp 71 (1982) 443
Louwrier, P.W.F., see E. Roduner 73 (1982) 117
Lu, P.Y., see Z.X. Yu 79 (1983) 289
Lucazeau, G., K. Chhor, C. Sourisseau and A.J. Dianoux, Neutron scattering study of the reorientational motions in $Cr(CO)_3(\eta^6C_6H_6)$ and $Mn(CO)_3(\eta^5C_5H_5)$ 76 (1983) 307
Luckhurst, G.R., S. Romano and P. Simpson, Computer simulation studies of anisotropic systems. IX. The Maier–Saupe theory for nematic liquid crystals and the molecular field approximation 73 (1982) 337
Luijks, G., J. Timmerman, S. Stolte and J. Reuss, Raman analysis of SF_6 molecular beams excited by a cw CO_2 laser 77 (1983) 169
Lund, A., see M. Tabata 75 (1983) 379
Luty, T., see R. Burzyński 72 (1982) 441
Lynch, D.W., see M. Piacentini 72 (1982) 61

MacLean, C., see W.P. Cofino 72 (1982) 73
Madzgalla, I., see K.-E. Süsse 78 (1983) 443
Mahieu, J.-P., see S. Evangelisti 75 (1983) 91
Maier, J.P., see D. Klapstein 72 (1982) 101
Maier, J.P., see S. Leutwyler 74 (1983) 441
Maier, J.P., see D. Klapstein 77 (1983) 463
Maier, J.P., see S. Leutwyler 78 (1983) 151
Maier, J.P., see D. Klapstein 78 (1983) 167
Makarov, V.I., N.L. Lavrik and N.M. Bazhin, Studies of magnetic field effects on the intensity and the lifetime of sulfur dioxide luminescence in the gas phase 72 (1982) 213
Mallett, C.P., see K. Norris 79 (1983) 9
Mallu, B.V., see Y.V. Chalapati Rao 74 (1983) 43
Malmquist, P.-Å., S. Svensson and H. Ågren, The N1s shake-up spectrum of para-aminobenzonitrile. A theoretical and experimental ESCA study 76 (1983) 429
Manocha, A.S., D.W. Setser and M.A. Wickramaaratchi, Vibrational energy disposal in reactions of fluorine atoms with hydrides of groups III, IV and V 76 (1983) 129
Manzanares, C., see V. Revelant 72 (1982) 224
Maraval, P., see J. Lascombe 72 (1982) 177
March, N.H., see J.A. Alonso 76 (1983) 121
March, N.H., see A.J. Easteal 76 (1983) 125
Marechal, Y., A quantitative analysis of the ν_s(IR) bands of H-bonds. I. Theory 79 (1983) 69
Marechal, Y., A quantitative analysis of the ν_s(IR) bands of H-bonds. II. Adipic acid crystals 79 (1983) 85
Margottin-Maclou, M., see F. Al Adel 74 (1983) 413
Marian, C.M., see B.A. Hess 71 (1982) 79
Marian, C.M., see R. Klotz 76 (1983) 367
Maricq, M.M., E.A. Gregory, C.T. Wickham-Jones, D.J. Cartwright and C.J.S.M. Simpson, Experimental and theoretical study of the vibrational relaxation of CO(v = 1) and N_2(v = 1): V–T relaxation by the isotopes of helium 75 (1983) 347
Maripuu, R., see I. Reineck 78 (1983) 311
Markey, B.R., see K. Norris 79 (1983) 9
Marletta, G., see O. Puglisi 75 (1983) 417
Martin, J.P., M.R. Buckingham, J.A. Chenery and C.J.S.M. Simpson, Relaxation of the individual vibrational levels of carbon monoxide following shock heating at 2100 K 74 (1983) 15
Martin, R.M., see M.S. de Vries 80 (1983) 157
Masci, D., see E. Borsella 77 (1983) 401
Maselko, J., Bifurcation diagrams for two substrate oscillatory systems 78 (1983) 381
Mathey, Y., see C. Sourisseau 71 (1982) 257
Mazurak, Z., J. Hanuza, K. Hermanowicz, B. Jeżowska- Trzebiatowska, D. Schultze and Ch. Waligora, Spectroscopic properties of Er^{3+} ions in Li(Er,Gs)P_4O_{12} single crystals – fluorescence, Raman and infrared spectra 79 (1983) 255
McAdoo, D.J., Comment on "Scaling relationships in photoelectron–photoion coincidence studies: the acetone ion dissociation" 80 (1983) 203
McAlpine, R.D., see D.K. Evans 80 (1983) 379
McCurdy, C.W., see J. Turner 71 (1982) 127
McDonald, J.R., see H.H. Nelson 73 (1982) 431
McDonald, J.R., see H.H. Nelson 74 (1983) 227
McDowell, H.K., Theoretical studies of ion neutralization: two-dimensional tight binding models 72 (1982) 451
McKeever, M.R., see S.J. Silvers 80 (1983) 177

McKenzie Jr., M.T. and E.R. Nixon, Fluorescence from the a ^{5}P and a ^{3}P states of matrix-isolated Fe atoms 75 (1983) 115
McLauchlan, K.A., see S. Basu 79 (1983) 95
McLeod, A., see R.T. Bailey 77 (1983) 243
McMahan, M.A., see M.M. Oprysko 79 (1983) 341
McMaster, B.N., J. Mrozek and V.H. Smith Jr., An ab initio molecular orbital study of the ammonium radical 73 (1982) 131
McMaster, B.N., see A. Pellegatti 75 (1983) 83
Meath, W.J., see R.A. Aziz 78 (1983) 295
Medvedev, E.S., The Franck–Condon principle for radiationless transitions in molecules and a selection rule for Morse oscillators 73 (1982) 243
Meech, S.R., D. Phillips and A.G. Lee, On the nature of the fluorescent state of methylated indole derivatives 80 (1983) 317
Meerts, W.L. and I. Ozier, Avoided-crossing molecular-beam spectroscopy of CH_3SiF_3 71 (1982) 401
Mehring, M., see W. Höptner 73 (1982) 253
Meiler, W., see Th. Weller 72 (1982) 155
Melzig, M., see G.J. Woolfe 77 (1983) 213
Messier, J., see P.-A. Chollet 73 (1982) 235
Mettes, J., see J. Tennyson 76 (1983) 195
Meyer, R., see G. Cirelli 72 (1982) 15
Meyer, W., see P. Botschwina 74 (1983) 321
Mialocq, J.C., Picosecond study of pinacyanol photophysics 73 (1982) 107
Michael, A., see Th. Weller 72 (1982) 155
Michel-Beyerle, M.E., see H.W. Krüger 74 (1983) 205
Michel-Beyerle, M.E., see W. Lersch 78 (1983) 115
Mikami, N., see M. Fujii 77 (1983) 191
Millar, D.P. and A.H. Zewail, Pulse substructure in passively and synchronously mode-locked cw dye lasers 72 (1982) 381
Miller, R.E., see G. Fischer 80 (1983) 147
Miller, R.J.D., R. Casalegno, K.A. Nelson and M.D. Fayer, Laser-induced ultrasonics: a dynamic holographic approach to the measurement of weak absorptions, optoelastic constants and acoustic attenuation 72 (1982) 371
Minchinton, A., C.E. Brion, J.P.D. Cook and E. Weigold, Molecular orbital electron momentum distributions and separation energies of CH_3CN 76 (1983) 89
Misev, L., see D. Klapstein 72 (1982) 101
Möbius, K., see W. Fröhling 75 (1983) 389
Moccia, R., see I. Cacelli 71 (1982) 199
Modelli, A., G. Distefano and D. Jones, Influence of the oxy, aza and thio groups on the electron affinities of carbonyl compounds studied by means of ETS 73 (1982) 395
Modelli, A., D. Jones, F.P. Colonna and G. Distefano, The nature of the stabilizing effect of thio groups on the Π anion states of benzene studied by means of electron transmission spectroscopy 77 (1983) 153
Moeller, Th., B. Jordan, P. Gürtler, G. Zimmerer, D. Haaks, J. le Calve and M.-C. Castex, Spectroscopic investigation of the electronic structure of the chlorine molecule in the VUV 76 (1983) 295
Mogensen, O.E., see G. Wikander 72 (1982) 407
Mogensen, O.E. and F.M. Jacobsen, Positronium yields in liquids determined by lifetime and angular correlation measurements 73 (1982) 223
Mogensen, O.E., see G. Wikander 77 (1983) 159

Mohamed, K.A., see G.N.A. van Veen 74 (1983) 261
Mohamed, K.A., see G.N.A. van Veen 80 (1983) 113
Molin, Yu.N., see A.B. Doktorov 71 (1982) 1
Monduzzi, M., see A. Lai 71 (1982) 271
Monti, S., G. Orlandi and P. Paimieri, Features of the photochemically active state surfaces of azobenzene 71 (1982) 87
Moraldi, M., Quantum-mechanical spectral moments in collision-induced light scattering and collision-induced absorption in rare gases at low densities 78 (1983) 243
Morand, P., see J. Moser 79 (1983) 277
Morokuma, K., see K. Ichikawa 72 (1982) 301
Morozov, I.I., see N.I. Butkovskaya 79 (1983) 21
Morra, B.S., see W. Höptner 73 (1982) 253
Morriss, G.P., see D.J. Evans 77 (1983) 63
Morsink, J.B.W., W.H. Hesselink and D.A. Wiersma, Photon echoes stimulated from long-lived ordered populations in multi-level systems. The effect of intersystem crossing and optical branching 71 (1982) 289
Moser, J., P. Morand, R. Duperrex and H. van den Bergh, Deuterium separation and infrared photochemistry in CF_2HCl 79 (1983) 277
Mrozek, J., see B.N. McMaster 73 (1982) 131
Mukherjee, D., see S. Ghosh 72 (1982) 161
Müller, J., L.J. Sæthre and O. Gropen, Molecular structure and photoelectron spectra of H_2S, H_2Se, and H_2Te. Effective core potential calculations on ground and valence ionic states 75 (1983) 395
Müller, W., see D. Eisel 80 (1983) 329
Munn, R.W., Electrostatic energy of vacancy formation in crystals of polar molecules 74 (1983) 301
Munn, R.W., see I. Eisenstein 74 (1983) 307
Munn, R.W., Unified theory of the electronic Stark effect in molecular crystals 76 (1983) 243
Munn, R.W., see D.A. Dunmur 76 (1983) 249
Munn, R.W., see I. Eisenstein 77 (1983) 47
Munn, R.W., see I. Eisenstein 79 (1983) 189

Nagata, T., T. Kondow and K. Kuchitsu, Polarization of CN($B\,^2\Sigma^+ - X\,^2\Sigma^+$) emission produced in the electron-impact dissociation of HCN and DCN 72 (1982) 281
Nagata, T., see Y. Ozaki 80 (1983) 73
Najbar, J., W. Jarzeba and Z.H. Urbanek, Internal heavy-atom effect on the T_1 states of monochloroquinolines and monochloronaphthalenes 79 (1983) 245
Nakagaki, R. and I. Hanazaki, Inequivalent methyl CH oscillators in methyl-substituted conjugated compounds as revealed by higher overtone spectra 72 (1982) 93
Nakajima, H., see H. Tanaka 75 (1983) 37
Nakamura, H., Semiclassical theory of predissociation induced by rotational (Coriolis) coupling 78 (1983) 235
Nakatsuji, H., Cluster expansion of the wavefunction. Valence and Rydberg excitations, ionizations and inner-valence ionizations of CO_2 and N_2O studied by the SAC and SAC CI theories 75 (1983) 425
Nakatsuji, H., see K. Ohta 76 (1983) 271
Nakatsuji, H., Cluster expansion of the wavefunction. Outer- and inner-valence ionization spectra of CS_2 and COS 76 (1983) 283
Nakatsuji, H., Cluster expansion of the wavefunction. Valence and Rydberg excitations, ionizations, and inner-valence ionizations of CO_2 and N_2O studied by the SAC and SAC CI theories, Chem. Phys. 75 (1983) 425. Erratum 80 (1983) 395
Nakatsuji, H., Cluster expansion of the wavefunction. Outer- and inner-valence ionization spectra of CS_2 and COS, Chem. Phys. 76 (1983) 283. Erratum 80 (1983) 395
Nascimento, M.A.C., The polarization dependence of two-photon absorption rates for randomly oriented molecules 74 (1983) 51
Natalis, P., P. Pennetreau, L. Longton and J.E. Collin, Autoionization in ClH and DCl by photoelectron spectroscopy 73 (1982) 191
Nauts, A. and X. Chapuisat, The description of molecular large-amplitude motions in terms of curvilinear coordinates associated with the reaction path 76 (1983) 349
Nedelec, O., see J. Dufayard 71 (1982) 279
Nelson, H.H., H. Helvajian, L. Pasternack and J.R. McDonald, Temperature dependence of $C_3(X\,^1\Sigma_g^+)$ reactions with alkenes and alkynes, 295–610 K 73 (1982) 431
Nelson, H.H., L. Pasternack and J.R. McDonald, Excitation and emission spectra of the $^2A_2'' \leftarrow\rightarrow {}^2E_1''$ system of the gas-phase cyclopentadienyl radical 74 (1983) 227
Nelson, K.A., see R.J.D. Miller 72 (1982) 371
Neubert, A. and K.F. Zmbov, The dissociation energies of gaseous SmLi, EuLi, TmLi and YbLi 76 (1983) 469
Nguyen, T.D. and N. Sadeghi, Rotational and vibrational distributions of $N_2(C\,^3\Pi_u)$ excited by state-selected $Ar(^3P_2)$ and $Ar(^3P_0)$ metastable atoms 79 (1983) 41
Nickel, B., see B. Dick 78 (1983) 1
Nickel, B., see D. Klemp 78 (1983) 17
Nigmatullin, R. and L.A. Dissado, Dipole–phonon coupling and dielectric relaxation 79 (1983) 455
Nikogosyan, D.N., A.A. Oraevsky and V.I. Rupasov, Two-photon ionization and dissociation of liquid water by powerful laser UV radiation 77 (1983) 131
Nishi, N., see M. Kawasaki 73 (1982) 377
Nishi, N., see M. Kawasaki 78 (1983) 65
Nishimura, Y., see H. Obase 74 (1983) 89
Nitzan, A., see B. Carmeli 72 (1982) 363
Nixon, E.R., see M.T. McKenzie Jr. 75 (1983) 115
Nobes, R.H. and L. Radom, A. theoretical study of the condensation reactions of methyl cation with ammonia, water, hydrogen fluoride and hydrogen sulphide 74 (1983) 163

Nohre, C., see I. Reineck 78 (1983) 311
Nomoto, K., see S. Tomoda 74 (1983) 113
NoorBatcha, I. and N. Sathyamurthy, Dynamics of a prototype alkali–hydrogen-halide exchange reaction on an ab initio potential-energy surface 77 (1983) 67
Nordholm, S., see H.W. Schranz 74 (1983) 365
Norris, K., P. Gray, D.P. Craig, C.P. Mallet and B.R. Markey, The effect of molecular excitation on crystal packing. 9-cyano- and 9,10-dimethylanthracene as excited guest/host and host/guest pairs 79 (1983) 9
Novak, A., see J. de Villepin 73 (1982) 291

Obase, H., M. Tsuji and Y. Nishimura, Energy-transfer reactions between He($2\,^3S$) and Ne($^3P_{0,2}$) metastable atoms and PN radicals 74 (1983) 89
Oddershede, J. and J.R. Sabin, X-ray scattering factors, Compton profiles, and shell corrections from numerical atomic wavefunctions 71 (1982) 161
Ogawa, T., see M. Higo 73 (1982) 99
Ogawa, Y., see M. Kawasaki 74 (1983) 83
Ohno, K., see S. Hino 71 (1982) 135
Ohta, K., H. Nakatsuji, H. Kubodera and T. Shida, Experimental and theoretical study on cation radicals of cyclopropane, cyclobutane and cyclopentane 76 (1983) 271
Oksengorn, B., see M. Châtelet 79 (1983) 413
Oliva, C., see M. Branca 75 (1983) 253
Olson, C.G., see M. Piacentini 72 (1982) 61
Oprysko, M.M., see F.J. Aoiz 79 (1983) 321
Oprysko, M.M., F.J. Aoiz, R.B. Bernstein and M.A. McMahan, Search for the laser-induced crossed beam reaction of excited I_2 ($B\,^3\Pi$) with Hg 79 (1983) 341
Oraevsky, A.A., see D.N. Nikogosyan 77 (1983) 131
Oref, I., see O. Herscovitz 71 (1982) 221
Orlandi, G., see S. Monti 71 (1982) 87
Osad'ko, I.S., see A.U. Jalmukhambetov 77 (1983) 247
Osamura, Y., Y. Yamaguchi, P. Saxe, M.A. Vincent, J.F. Gaw and H.F. Schaefer III, Unified theoretical treatment of analytic first and second energy derivatives in open-shell Hartree–Fock theory 72 (1982) 131
Otten, D., see U. Buck 77 (1983) 201
Ottinger, Ch., J. Reichmuth and M. Yang, Luminescent charge transfer of ground-state and metastable B^+ ions 76 (1983) 61
Ovchinnikov, A.A., see Yu.I. Dakhnovskii 80 (1983) 17
Owyoung, A., see P. Esherick 73 (1982) 271
Ozaki, Y., T. Kondow and K. Kuchitsu, Dynamics of formation of CN($B\,^2\Sigma^+$) fragment from HCN and DCN in argon afterglow 77 (1983) 223
Ozaki, Y., T. Nagata, K. Suzuki, T. Kondow and K. Kuchitsu, Rotational perturbations in the CN ($B\,^2\Sigma^+$–$X\,^2\Sigma^+$) tail band system. I. Analysis of the $v = 27$ and 30 levels of CN ($A\,^2\Pi_i$) 80 (1983) 73
Ozaki, Y., H. Ito, K. Suzuki, T. Kondow and K. Kuchitsu, Rotational perturbations in the CN ($B\,^2\Sigma^+$–$X\,^2\Sigma^+$) tail band system. II. Identification of the CN ($^4\Pi$) state and its vibrational levels 80 (1983) 85
Ozier, I., see W.L. Meerts 71 (1982) 401

Pacchioni, G. and J. Koutecký, The bond nature of alkaline-earth homonuclear metal clusters investigated with pseudopotential CI method 71 (1982) 181
Pacynko, W.F., J. Yarwood and D.J. Gardiner, Raman spectroscopic studies on the dynamics of a molecular "probe" (methyl iodide) in hydrocarbon solvents 78 (1983) 319
Pagel, M., see P. Tola 78 (1983) 339
Paidarová, I., J. Vojtík and R. Polák, Atoms-in-molecules calculations on diatomic fragments of polyatomic systems: HeH, HeH^+ and HeH^- for a DIM model of Penning ionization of H_2 by He^* 72 (1982) 119
Paliani, G., see R. Cataliotti 72 (1982) 293
Palmer, M.H., F.E. Scott and J.A.S. Smith, Calculation of the ^{14}N and ^2H quadrupole coupling tensor in trimeric imidazole 74 (1983) 9
Palmieri, P., see S. Monti 71 (1982) 87
Parker, D.H., see S. Stolte 71 (1982) 353
Parlant, G., M. Schröder and S. Goursaud, Trajectory surface-hopping study of the $K + O_2$ collision: energy transfer in neutral and ionic products 75 (1983) 175
Parr, A.C., see J. Dannacher 75 (1983) 23
Pasimeni, L., see G. Agostini 77 (1983) 233
Pasternack, L., see H.H. Nelson 73 (1982) 431
Pasternack, L., see H.H. Nelson 74 (1983) 227
Patel, J.S. and D.M. Hanson, Photochemical control of energy transfer in molecular crystals 72 (1982) 35
Pattengill, M.D., Classical trajectory study of three-body direct photofragmentation of $Cd(CH_3)_2$. Comparison of sampling methods 75 (1983) 59.
Pattengill, M.D., Classical trajectory study of the effects of parent-molecule bending and overall rotation in polyatomic direct photofragmentation. Model $ICN + h\nu \rightarrow CN + I$ 78 (1983) 229
Peau, E.W., see M. Winnewisser 71 (1982) 377
Pedersen, N.-J., see G. Wikander 77 (1983) 159
Pei, C.-C., see K.-M. Chen 76 (1983) 219
Pellegatti, A., B.N. McMaster and D.R. Salahub, Electronic structure of potassium clusters (K_9, K_{15}, K_{27}) by the SCF Xα(LSD) SW method 75 (1983) 83
Pennetreau, P., see P. Natalis 73 (1982) 191
Percival, I.C., see S.M. Colwell 75 (1983) 215
Percival, I.C., see S.M. Colwell 75 (1983) 225
Perrin, J., J.P.M. Schmitt, G. de Rosny, B. Drevillon, J. Huc and A. Lloret, Dissociation cross sections of silane and disilane by electron impact 73 (1982) 383
Perrin, J. and J.F.M. Aarts, Dissociative excitation of SiH_4, SiD_4, Si_2H_6 and GeH_4 by 0–100 eV electron impact 80 (1983) 351
Peter, G., see L. Sebastian 75 (1983) 103
Peter, G., B. Ries and H. Bässler, Singlet exciton migration in a random organic two-component system containing physical and chemical traps 80 (1983) 289
Petrella, G., see F.A. Gianturco 78 (1983) 81
Petrochenko, S.I., see M.V. Basilevsky 72 (1982) 349
Pettersson, L.G.M., U. Wahlgren and O. Gropen, Effective core potential calculations using frozen orbitals. Applications to transition metals 80 (1983) 7
Peyerimhoff, S.D., see B.A. Hess 71 (1982) 79
Peyerimhoff, S.D. and R.J. Buenker, Potential energy curves and transition moments for the low-lying electronic states of the Si_2 molecule 72 (1982) 111
Peyerimhoff, S.D., see P.G. Burton 73 (1982) 83
Peyerimhoff, S.D., see R. Klotz 76 (1983) 367

Pfeiffer, M., see Ch. Jung 72 (1982) 327
Phillies, G.D.J., Non-hydrodynamic contribution to the concentration dependence of the self diffusion of interacting brownian macroparticles 74 (1983) 197
Phillips, D., see P.C. Alford 76 (1983) 103
Phillips, D., see S.R. Meech 80 (1983) 317
Piacentini, M., F.S. Khumalo, G. Leveque, C.G. Olson and D.W. Lynch, X-ray photoemission and optical spectra of $NiPS_3$, $FePS_3$ and $ZnPS_3$ 72 (1982) 61
Piaggio, P., G. Dellepiane, R. Tubino and L. Piseri, Fermi resonance and bandshapes in deuterated palmitic acid 77 (1983) 185
Pignataro, S., see O. Puglisi 75 (1983) 417
Piseri, L., see P. Piaggio 77 (1983) 185
Poinsignon, C., see C. Sourisseau 71 (1982) 257
Polák, R., see I. Paidarová 72 (1982) 119
Polák, R., see F. Schneider 76 (1983) 259
Polák, R. and J. Vojtík, Atoms-in-molecules study of ground- and excited-state potential-energy curves for Li_2 78 (1983) 107
Polanyi, J.C., see P. Arrowsmith 79 (1983) 31
Ponte Goncalves, A.M., see R. Gillies 78 (1983) 49
Pople, J.A., see M.J. Frisch 75 (1983) 323
Poquet, E., see H. Cardy 77 (1983) 287
Port, H., see D. Rund 78 (1983) 357
Potthast, L., see M. Hoffmeister 78 (1983) 369
Poulsen, L.L. and G.D. Billing, Vibrational deactivation of CO(v = 1) by p-H_2 and o-H_2 73 (1982) 313
Powis, I., The unimolecular dissociation of electronic state-selected methyl iodide cations 74 (1983) 421
Preuss, H., see J. Flad 75 (1983) 331
Pritchard, H.O. and S.R. Vatsya, On the connection between incubation and relaxation times in thermal unimolecular reactions 72 (1982) 447
Pryor, A.W., see J.E. Eberhardt 72 (1982) 41
Pryor, A.W., see J.E. Eberhardt 72 (1982) 51
Puebla, C., see A. Schönhofer 76 (1983) 453
Pugh, D., see R.T. Bailey 77 (1983) 243
Puglisi, O., G. Marletta, S. Pignataro and G. Foti, Reactions induced by ion bombardment of solid cyclohexane at 77 K 75 (1983) 417
Pyda, M. and M. Kurzyński, Theory of sorption of gases on polymers. II. Effects of inter-chain secondary bonds 79 (1983) 219
Pyykkö, P., see A. Viste 72 (1982) 225
Pyykkö, P., see R.G. Egdell 72 (1982) 237
Pyykkö, P., On the relativistic theory of NMR chemical shifts 74 (1983) 1

Rabinovitch, B.S., see S.P. Wrigley 75 (1983) 453
Raczyński, A., Collision-induced absorption in a He–Ar mixture 72 (1982) 321
Rademann, K., B. Brutschy and H. Baumgärtel, Electronic spectroscopy of fluorobenzene van der Waals molecules by resonant two-photon ionization 80 (1983) 129
Radom, L., see R.H. Nobes 74 (1983) 163
Radom, L., see M.J. Frisch 75 (1983) 323
Raghavachari, K., see M.J. Frisch 75 (1983) 323
Raitsimring, A.M. and V.V. Tregub, Electron spin echo decay kinetics of an ion track in β-irradiated frozen solution of sulfuric acid. Numerical simulation by the Monte Carlo method and experiment 77 (1983) 123
Rákóczi, F.J., T.-K. Ha and Hs.H. Günthard, Detection and identification of free radicals in the gaseous-phase ozonolysis of ethylene: microreactor–matrix ESR spectroscopy 74 (1983) 273
Ramaker, D.E., Comparison of photon-stimulated dissociation of gas-phase, solid and chemisorbed water 80 (1983) 183
Ramaswamy, R., Chaotic motions in vibrating molecules: the generalized Hénon–Heiles model 76 (1983) 15
Rao, C.N.R., see D.D. Sarma 73 (1982) 71
Rao, C.N.R., see G. Sankar 76 (1983) 435
Ravenek, W., J.W.M. Jacobs and A. van der Avoird, Hartree–Fock–Slater LCAO calculation of the Mössbauer parameters of some antimony compounds 78 (1983) 391
Rayner, D.M., S. Kimel and P.A. Hackett, The nascent translational energy of difluorocarbene produced in IR MPD of the pentafluoroethyl radical 77 (1983) 349
Reichmuth, J., see Ch. Ottinger 76 (1983) 61
Reimschüssel, W., H. Abramczyk, H. Barańska and A. Łabudzinska, Raman Scattering study of toluene vibrational relaxation in benzene–toluene liquid system 72 (1982) 313
Reineck, I., C. Nohre, R. Maripuu, P. Lodin, S.H. Al-Shamma, H. Veenhuizen, L. Karlsson and K. Siegbahn, High-resolution UV photoelectron spectrum of CO_2 78 (1983) 311
Renn, A., see M. Brieger 75 (1983) 1
Retournard, A., see P. Tola 78 (1983) 339
Rettrup, S., see H. Johansen 74 (1983) 77
Reuss, J., to Tony Dymanus, born 6th August 1922 in Janowice, Poland 71 (1982) 307
Reuss, J., see G. Luijks 77 (1983) 169
Revelant, V. and C. Manzanares I, Theoretical probabilities of V–V energy transfer: CO with isotopes of N_2 and deactivation of laser-excited SO_2, Chem. Phys. 69 (1982) 473. Erratum 72 (1982) 224
Ries, B., see G. Peter 80 (1983) 289
Righini, R., see R.G. Della Valle 74 (1983) 179
Riley, M.J., A.R. Lacey, M.G. Sceats and R.G. Gilbert, Low-temperature vibronic spectra of 1,1′-binaphthyl 72 (1982) 83
Ritchie, A.J.D., see S. Basu 79 (1983) 95
Roduner, E., G.A. Brinkman and P.W.F. Louwrier, Muonium-substituted organic free radicals in liquids. Muon–electron hyperfine coupling constants and the selectivity of formation of methyl- and fluorine-substituted cyclohexadienyl-type radicals 73 (1982) 117
Rohmer, M.-M., A. Dedieu and A. Veillard, Structure and properties of a model of deoxyheme. An ab initio SCF calculation 77 (1983) 449
Romano, S., see G.R. Luckhurst 73 (1982) 337
Römelt, J., Prediction and interpretation of collinear reactive scattering resonances by the diagonal corrected vibrational adiabatic hyperspherical model 79 (1983) 197
Roos, B.O., see G.H.F. Diercksen 77 (1983) 93
Root, J.H., see P.A. Egelstaff 76 (1983) 405

Rösch, N., Time-reversal symmetry, Kramers' degeneracy and the algebraic eigenvalue problem 80 (1983) 1
Rosenstock, H.M., see J. Dannacher 75 (1983) 23
Rosmus, P., see H.-J. Werner 73 (1982) 169
Rudny, E.B., see L.N. Sidorov 71 (1982) 145
Ruedenberg, K., M.W. Schmidt, M.M. Gilbert and S.T. Elbert, Are atoms intrinsic to molecular electronic wavefunctions? I. The FORS model 71 (1982) 41
Ruedenberg, K., M.W. Schmidt and M.M. Gilbert, Are atoms intrinsic to molecular electronic wavefunctions? II. Analysis of FORS orbitals 71 (1982) 51
Ruedenberg, K., M.W. Schmidt, M.M. Gilbert and S.T. Elbert, Are atoms intrinsic to molecular electronic wavefunctions? III. Analysis of FORS configurations 71 (1982) 65
Rund, D. and H. Port, Triplet-state optical spectra of highly concentrated isotopically mixed crystals of anthracene A-h_{10}:A-d_{10} 78 (1983) 357
Rupasov, V.I., see D.N. Nikogosyan 77 (1983) 131
Russo, N., see V. Barone 76 (1983) 385
Rynefors, K. and L. Holmlid, Monte Carlo simulation of RRKM unimolecular decomposition in molecular beam experiments. II. Application to angular distributions and absolute cross sections for the system K + RbCl, Chem. Phys. 60 (1981) 405. Erratum 74 (1983) 446
Ryzlewicz, Ch., H.-U. Schütze-Pahlmann, J. Hoeft and T. Törring, Rotational spectrum and hyperfine structure of the $^2\Sigma$ radicals BaF and BaCl 71 (1982) 389

Saba, G., see A. Lai 71 (1982) 271
Sabin, J.R., see J. Oddershede 71 (1982) 161
Sadeghi, N., see T.D. Nguyen 79 (1983) 41
Sadlej, A.J., see G.H.F. Diercksen 71 (1982) 105
Sadlej, A.J., see G.H.F. Diercksen 77 (1983) 93
Sadlej, A.J., see G.H.F. Diercksen 77 (1983) 429
Sæthre, L.J., see J. Müller 75 (1983) 395
Sage, M.L. and J. Jortner, Two-photon excitations of bond modes 72 (1982) 249
Saha, S.K., see B.C. Khanra 76 (1983) 255
Saito, G., see N. Sato 76 (1983) 79
Sakimoto, K., A comparison of quantal and semiclassical perturbed-rotational-state methods in H^+–CO collisions 79 (1983) 137
Salahub, D.R., see A. Pellegatti 75 (1983) 83
Samanta, L.K., D.K. Ghosh and G.C. Bhar, Band-state interpretation of lattice thermal conductivity and microhardness of ternary chalcopyrite semiconductors 79 (1983) 361
Sams, J.R., see J.S. Haynes 78 (1983) 127
Sankar, G., P.R. Sarode and C.N.R. Rao, A XANES study of mixed-valence transition-metal oxides and rare-earth alloys 76 (1983) 435
Sanna, G., see C. di Lauro 73 (1982) 215
Sarma, D.D., P. Vishnu Kamath and C.N.R. Rao, Satellites in the X-ray photoelectron spectra of transition-metal and rare-earth compounds 73 (1982) 71
Sarode, P.R., see G. Sankar 76 (1983) 435
Sathyamurthy, N., see I. NoorBatcha 77 (1983) 67
Sato, H., see M. Kawasaki 73 (1982) 377
Sato, H., see M. Kawasaki 74 (1983) 83
Sato, H., see M. Kawasaki 78 (1983) 65
Sato, K., see S. Tomoda 74 (1983) 113
Sato, N., G. Saito and H. Inokuchi, Ionization potentials and polarization energies of tetraselenafulvalene (TSF) derivatives determined from ultraviolet photoelectron spectroscopy 76 (1983) 79
Saunders, V.R., see A. Laaksonen 80 (1983) 221
Saxe, P., see Y. Osamura 72 (1982) 131
Sazonov, V.N. and I.E. Khromov, On the statistics of an ensemble of oscillators under excitation. IV. Evaluation of the time for kinetic excitation into the quasicontinuum based on Kramers' theory 76 (1983) 25
Sceats, M.G., see M.J. Riley 72 (1982) 83
Schaefer III, H.F., see Y. Osamura 72 (1982) 131
Schatz, G.C., see L.C. Geiger 79 (1983) 431
Schermann, J.P., see J.P. Astruc 75 (1983) 405
Schiller, J., see J. Hormes 74 (1983) 433
Schinke, R., see D. Häusler 79 (1983) 147
Schirmer, J. and O. Walter, Complete valence-shell ionization spectra of N_2 and CO: application of the extended two-particle–hole Tamm–Dancoff approximation (2ph-TDA) 78 (1983) 201
Schlier, Ch.G., Collinear collisions in a well potential 77 (1983) 257
Schmid, D., see R. Krauss 73 (1982) 55
Schmidt, M.W., see K. Ruedenberg 71 (1982) 41
Schmidt, M.W., see K. Ruedenberg 71 (1982) 51

Schmidt, M.W., see K. Ruedenberg 71 (1982) 65
Schmitt, J.P.M., see J. Perrin 73 (1982) 383
Schmitz, K.S., Quasi-elastic light scattering studies on T7 DNA in the presence of a sinusoidal electric field 79 (1983) 297
Schneider, F., L. Zülicke, R. Polák and J. Vojtík, Diatomics-in-molecules potential energy surfaces of $(HeH_2)^+$: an extended basis set calculation 76 (1983) 259
Schneider, S., G.J. Woolfe 77 (1983) 213
Schönhofer, A., H.-G. Kuball and C. Puebla, Optical activity of oriented molecules. IX. Phenomenological Mueller matrix description of thick samples and of optical elements 76 (1983) 453
Schott, M., see J. Berréhar 77 (1983) 11
Schranz, H.W. and S. Nordholm, An efficient solution of weak-collision master equations in thermal unimolecular reaction rate theory 74 (1983) 365
Schreiner, W. and K.W. Kratky, Influence of box shape on the hard-disk pressure at high fluid density 80 (1983) 245
Schriever, J., see D. Lankhorst 77 (1983) 319
Schröder, J.O., see W.E. Ernst 78 (1983) 363
Schröder, M., see G. Parlant 75 (1983) 175
Schrof, W., see R. Krauss 73 (1982) 55
Schultze, D., see Z. Mazurak 79 (1983) 255
Schulze, W., see W. Vogel 74 (1983) 137
Schurr, J.M., The fluctuating-force formulation of friction drag coefficients 71 (1982) 101
Schütze-Phalmann, H.-U., see Ch. Ryzlewicz 71 (1982) 389
Scoles, G., see D. Bassi 71 (1982) 239
Scotoni, M., see D. Bassi 71 (1982) 239
Scott, F.E., see M.H. Palmer 74 (1983) 9
Sebastian, L., G. Weiser, G. Peter and H. Bässler, Charge-transfer transitions in crystalline anthracene and their role in photoconductivity 75 (1983) 103
Seki, K., see S. Hino 71 (1982) 135
Senn, P., see P.R. Keller 74 (1983) 247
Sergeev, P.A. and D.I. Slovetsky, Vibrationally excited molecules and mechanisms of chemical and physical processes in non-equilibrium plasmas 75 (1983) 231
Setser, D.W., see A.S. Manocha 76 (1983) 129
Sexton, G.J., see P.J. Knowles 72 (1982) 337
Shapiro, M., see G.G. Balint-Kurti 72 (1982) 456
Shibuya, K. and F. Stuhl, Fluorescence lifetime and collisional quenching of the predissociative NO $B\,^2\Pi$ ($v' = 7$) state 79 (1983) 367
Shida, T., see K. Ohta 76 (1983) 271
Shinohara, H., see M. Kawasaki 73 (1982) 377
Shinohara, H., see M. Kawasaki 78 (1983) 65
Shirk, J.S., see W.F. Hoffman III 78 (1983) 331
Shizgal, B. and R. Blackmore, Eigenvalues of the Boltzmann collision operator for binary gases: relaxation of anisotropic distributions 77 (1983) 417
Sidorov, L.N., A.Ya. Borshchevsky, E.B. Rudny and V.D. Butsky, Electron affinities of higher molybdenum fluorides as determined by the effusion technique 71 (1982) 145
Siebrand, W. and M.Z. Zgierski, Vibronic and multimode effects on the Raman excitation profile of a totally symmetric fundamental in the Soret band of cytochrome **c** 77 (1983) 35
Siegbahn, K., see I. Reineck 78 (1983) 311
Siegbahn, P.E.M., see M. Larsson 76 (1983) 175

Siegel, D., H. Sixl, V. Enkelmann and G. Wenz, Polymerization of TS-12 diacetylene crystals: crystal structures of monomer and polymer and spectroscopy of reaction intermediates 72 (1982) 201
Silvers, S.J., M.R. McKeever and G.K. Chawla, The effect of a magnetic field on discrete and continuum CS_2 fluorescence 80 (1983) 177
Simonetta, M., see M. Branca 75 (1983) 253
Simpson, C.J.S.M., see J.P. Martin 74 (1983) 15
Simpson, C.J.S.M., see M.M. Maricq 75 (1983) 347
Simpson, C.J.S.M., see D.C. Allen 76 (1983) 231
Simpson, P., see G.R. Luckhurst 73 (1982) 337
Singh, J., Comparative reinvestigation of the interaction of phonons with Wannier and Frenkel excitons in crystalline solids 75 (1983) 371
Sipp, B., Hopping transport and energy transfer in substitutionally disordered media 77 (1983) 257
Sixl, H., see D. Siegel 72 (1982) 201
Sixl, H., see D. Higelin 77 (1983) 391
Skodje, R.T., W.R. Gentry and C.F. Giese, Quantum vibrational transition probabilities from real classical trajectories: asymmetric diatom–diatom collisions 74 (1983) 347
Slovetsky, D.I., see P.A. Sergeev 75 (1983) 231
Smith, D.R., see J.S. Geiger 74 (1983) 239
Smith, J.A.S., see M.H. Palmer 74 (1983) 9
Smith, K.W., see S.P. Wrigley 75 (1983) 453
Smith Jr., V.H., see B.N. McMaster 73 (1982) 131
Smulevich, G., A. Amirav, U. Even and J. Jortner, Electronic–vibrational excitations of a hydrogen-bonded molecule in supersonic expansions: 1,4-dihydroxyanthraquinone and its deuterated derivatives 73 (1982) 1
Smulevich, G., A. Amirav, U. Even and J. Jortner, Electronic–vibrational excitations of a hydrogen-bonded molecule in supersonic expansions: 1,4-dihydroxyanthraquinone and its deuterated derivatives, Chem. Phys. 73 (1982) 1. Erratum 76 (1983) 147
Snijders, J.G., see R.G. Egdell 72 (1982) 237
Sobolewski, A.L., Non-Condon scheme of radiationless transitions for the Morse oscillator model 78 (1983) 265
Sodeik, A., see M. Brieger 75 (1983) 1
Solgadi, D., F. Lahmani, C. Lardeux and J.P. Flament, Ab initio CI study of the photodissociation of nitrosyl chloride (ClNO) 79 (1983) 225
Solodovnikov, G.A., see V.V. Likhansky 77 (1983) 409
Sontag, H., B. Eberle and R. Weber, Matrix-isolation spectroscopy of Pb_2 80 (1983) 279
Sorriso, S., see H.A. Kołodziej 77 (1983) 341
Sorriso, S., see H.A. Kołodziej 78 (1983) 75
Sourisseau, C., Y. Mathey and C. Poinsignon, Inelastic neutron scattering study of low frequency motions in $[Co(C_5H_5)_2^+]$ and $[Cr(C_6H_6)_2^+]$ intercalated in the $MnPS_3$ layered compound 71 (1982) 257
Sourisseau, C., see G. Lucazeau 76 (1983) 307
Spinelli, D., See G. Distefano 72 (1982) 267
Stadelmann, J.-P., see R. Bombach 72 (1982) 259
Stadelmann, J.-P., see J. Dannacher 75 (1983) 23
Staemmler, V., see K. Kaufmann 79 (1983) 111
Steele, W.A., see S. Gupta 72 (1982) 425
Steinberg, I.Z., see J. Anglister 75 (1983) 443
Steinhauser, O., On the structure and dynamics of liquid benzene 73 (1982) 155

Steinhauser, O., On the dielectric theory and computer simulation of water 79 (1983) 465
Stephan-Rossbach, K.-H. and F.J. Comes, New I_2 emission from iodine atom recombination reaction 80 (1983) 121
Stockbauer, R.L., see J. Dannacher 75 (1983) 23
Stoll, H., see J. Flad 75 (1983) 331
Stolte, S., K.K. Chakravorty, R.B. Bernstein and D.H. Parker, Analysis of the steric dependence of the CH_3I + Rb reaction using a Legendre expansion technique 71 (1982) 353
Stolte, S., see G. Luijks 77 (1983) 169
Stuhl, F., see K. Shibuya 79 (1983) 367
Subra, R., see V. Barone 76 (1983) 385
Sugawara, Y., see K. Ichikawa 72 (1982) 301
Sundström, V., T. Gillbro and H. Bergström, Picosecond kinetics of radiationless relaxation of triphenyl methane dyes. Evidence for rapid excited-state equilibrium between states of differing geometry 73 (1982) 439
Süsse, K.-E., D.-G. Welsch and I. Madzgalla, Viscosity dependence of internal conversion rates of polyatomic molecules 78 (1983) 443
Suter, G.W. and U.P. Wild, The dual phosphorescence of benzophenazine in ethanol 73 (1982) 421
Suzuki, K., see Y. Ozaki 80 (1983) 73
Suzuki, K., see Y. Ozaki 80 (1983) 85
Svensson, S., see P.-Å. Malmquist 76 (1983) 429

Tabata, M. and A. Lund, Structure and photodecomposition reactions of cations of cyclopentane, cyclohexane, cyclic olefines and dienes in γ-irradiated frozen solutions of CF_3CCl_3. An ESR study 75 (1983) 379
Takeuchi, H. and M. Tasumi, Infrared-induced conformational isomerization of ethylene glycol in a low-temperature argon matrix 77 (1983) 21
Tal'rose, V.L., see N.I. Butkovskaya 79 (1983) 21
Tanaka, H., Y. Wada and H. Nakajima, Acoustic study of a critical binary mixture of nitrobenzene and *n*-hexane at low and ultrasonic frequencies 75 (1983) 37
Tanaka, H. and Y. Wada, Adiabatic compressibility of critical binary mixtures of nitroethane/isooctane and nitroethane/3-methylpentane 78 (1983) 143
Tasumi, M., see H. Takeuchi 77 (1983) 21
Taylor, J.W., see P.R. Keller 74 (1983) 247
Taylor, J.W., see P.R. Keller 79 (1983) 269
Taylor, P.R., see R. Ahlrichs 72 (1982) 287
Telle, H.H., see P. Arrowsmith 79 (1983) 31
Tennyson, J. and J. Mettes, Calculated ro-vibrational fine-structure spectrum and weak-field Zeeman splittings of the O_2Ar van der Waals molecule 76 (1983) 195
Ter Haar, D., Turbulence in fluids and plasmas 71 (1982) 345
Tesche, B., see W. Vogel 74 (1983) 137
Thiel, W., Theoretical analysis of photoelectron angular distributions of linear molecules 77 (1983) 103
Thole, B.T. and P.Th. van Duijnen, The direct reaction field hamiltonian: analysis of the dispersion term and application to the water dimer 71 (1982) 211
Thompson, R.C., see J.S. Haynes 78 (1983) 127
Thuler, M.R., R.L. Benbow and Z. Hurych, Synchrotron-radiation photoemission study of the V–VI layered compounds Bi_2Te_3, Bi_2Se_3, Sb_2Te_3 and Sb_2Te_2Se 71 (1982) 265
Tiffon, B., see B. Ancian 74 (1983) 171
Timmerman, J., see G. Luijks 77 (1983) 169
Toennies, J.P., see T. Ellenbroek 71 (1982) 309
Toennies, J.P., see G. Drolshagen 79 (1983) 159
Tokue, I. and Y. Ito, Formation of HN ($A\,^3\Pi$, $c\,^1\Pi$) by electron-impact dissociation of HN_3 79 (1983) 383
Tola, P., A. Retournard, J. Dexpert-Ghys, M. Lemonnier, M. Pagel and J. Coulon, On the use of X-ray-excited optical luminescence (XEOL) for the analysis of multisite rare-earth systems 78 (1983) 339
Tola, P., see J. Goulon 78 (1983) 347
Tolkatchev, V.A., see V.L. Vyazovkin 75 (1983) 11
Tolkatchev, V.A., see V.A. Bagryansky 78 (1983) 41
Tomkinson, J., see J. Howard 77 (1983) 145
Tomoda, S., Y. Achiba, K. Nomoto, K. Sato and K. Kimura, Photoelectron spectroscopic study of simple hydrogen-bonded dimers. I. Supersonic nozzle beam photoelectron spectrometer and the formic-acid dimer 74 (1983) 113
Tomoda, S. and K. Kimura, Photoelectron spectroscopic study of simple hydrogen-bonded dimers. II. The methanol dimer 74 (1983) 121
Törring, T., see Ch. Ryzlewicz 71 (1982) 389
Tosi, M.P., see A.J. Easteal 76 (1983) 125
Trabjerg, I., see J. Baiardo 79 (1983) 391
Trabjerg, I., see J. Baiardo 80 (1983) 305
Trachtman, M., see C.W. Bock 73 (1982) 179
Tregub, V.V., see A.M. Raitsimring 77 (1983) 123

Truong, T.B., Charge transfer to a solvent state. VIII. Localization of charge during the transition state of the solute: the solute cation localization energy 77 (1983) 377
Tse, J.S., see D.J. Bristow 75 (1983) 263
Tse, J.S., see G.M. Bancroft 75 (1983) 277
Tso, T.-L., see M. Diem 73 (1982) 283
Tsuboi, M., see K. Ichikawa 72 (1982) 301
Tsuji, M., see H. Obase 74 (1983) 89
Tubino, R., see P. Piaggio 77 (1983) 185
Tulman, R., see B. Carmeli 72 (1982) 363
Turner, J. and C.W. McCurdy, The application of exterior complex scaling in calculations on resonances in nuclear motion in molecular systems 71 (1982) 127
Tzidoni, E., see O. Herscovitz 71 (1982) 221

Urbanek, Z.H., see J. Najbar 79 (1983) 245
Uzhinov, B.M., see S.I. Druzhinin 78 (1983) 29

Vala, M., see J. Baiardo 79 (1983) 391
Vala, M., see J. Baiardo 79 (1983) 403
Vala, M., see J. Baiardo 80 (1983) 305
Van den Bergh, H., see J. Moser 79 (1983) 277
Van der Avoird, A., see W. Ravenek 78 (1983) 391
Van der Kam, P.M.A., see H.C.W. Beijerinck 72 (1982) 391
Van Dishoeck, E.F., Oscillator strengths and lifetimes of the $C_2A\,^1\Pi_u$–$X\,^1\Sigma_g^+$ Phillips system 77 (1983) 277
Van Duijnen, P.Th., see B.T. Thole 71 (1982) 211
Van Veen, G.N.A., K.A. Mohamed, T. Baller and A.E. de Vries, Photofragmentation of H_2S in the first continuum 74 (1983) 261
Van Veen, G.N.A., K.A. Mohamed, T. Baller and A.E. de Vries, Photofragmentation of III in the first continuum 80 (1983) 113
Vasiliev, E.S., see N.I. Butkovskaya 79 (1983) 21
Vatsya, S.R., see H.O. Pritchard 72 (1982) 447
Veenhuizen, H., see I. Reineck 78 (1983) 311
Veillard, A., see M.-M. Rohmer 77 (1983) 449
Velthorst, N.H., see W.P. Cofino 72 (1982) 73
Venkatesh, S., see R.T. Bailey 77 (1983) 243
Verster, N.F., see H.C.W. Beijerinck 72 (1982) 391
Veszprémi, T., see S. Hino 71 (1982) 135
Viehland, L.A., Interaction potentials for Li^+–rare-gas systems 78 (1983) 279
Villaeys, A.A. and K.F. Freed, Time-resolved spectroscopy: wavepacket formalism in the coherent-state representation 72 (1982) 1
Vincent, M.A., see Y. Osamura 72 (1982) 131
Vishnu Kamath, P., see D.D. Sarma 73 (1982) 71
Viste, A., M. Hotokka, L. Laaksonen and P. Pyykkö, Relativistically parameterized extended Hückel calculations. VII. Nuclear spin–spin coupling tensors and densities of states for cluster models of CdTe, HgTe and PbTe 72 (1982) 225
Vogel, W., B. Tesche and W. Schulze, X-ray structure and optical properties of silver films prepared by condensation of pre-formed Ag-clusters 74 (1983) 137
Vogt, J., see R. Bombach 72 (1982) 259
Vojtík, J., see I. Paidarová 72 (1982) 119
Vojtík, J., see F. Schneider 76 (1983) 259
Vojtík, J., see R. Polák 78 (1983) 107
Von Schütz, J.U., see W. Höptner 73 (1982) 253
Vyazovkin, V.L., B.V. Bol'shakov and V.A. Tolkatchev, Kinetics of methyl radial reaction with methanol at 20–105 K 75 (1983) 11

Wada, Y., see H. Tanaka 75 (1983) 37
Wada, Y., see H. Tanaka 78 (1983) 143
Wahlgren, U., see L.G.M. Pettersson 80 (1983) 7
Waligora, Ch., see Z. Mazurak 79 (1983) 255
Wallace, R., The selection of coordinate systems for describing large-amplitude nuclear motion in triatomic molecules 71 (1982) 173
Wallace, R., Large-amplitude vibration in triatoms. II. Introduction of potential refinement within a LAV model applied to the sulfur dioxide molecule 74 (1983) 339
Wallace, R., Large-amplitude vibration in triatoms. III. Application to linear molecules: vibrational states of HCN 76 (1983) 421
Walter, O., see J. Schirmer 78 (1983) 201
Warman, J.M., see M.P. de Haas 73 (1982) 35
Watson, T.A., M. Addison and C. Wittig, Photolytic production of $O(^3P)$ in the presence of CF_3I: the formation of $IF(X\,^1\Sigma^+)$ 78 (1983) 57
Watts, R.O., see G. Fischer 80 (1983) 147
Waugh, A.B., see J.E. Eberhardt 72 (1982) 41
Weber, R., see H. Sontag 80 (1983) 279
Wegner, G., see W. Höptner 73 (1982) 253
Weigmann, H.-J., see Ch. Jung 72 (1982) 327
Weigold, E., see A. Minchinton 76 (1983) 89
Weinert, C.M., F. Forstmann, R. Grinter and D.M. Kolb, On the role of the dynamic Jahn–Teller effect in the spectra of matrix-isolated atoms with strong spin–orbit coupling 80 (1983) 95
Weiser, G., see L. Sebastian 75 (1983) 103
Weller, Th., W. Meiler, A. Michael, H.J. Köhler, H. Lischka and R. Höller, Ab initio calculation of the equilibrium geometry and the ^{13}C, ^{17}O and ^{27}Al NMR chemical shielding tensors of the system Al^{3+}/CO 72 (1982) 155
Welsch, D.-G., see K.-E. Süsse 78 (1983) 443
Wenz, G., see D. Siegel 72 (1982) 201
Werncke, W., see Ch. Jung 72 (1982) 327
Werner, H.-J., P. Rosmus and M. Grimm, Ab initio calculations of radiative transition probabilities in the $X\,^1\Sigma^+$ state of SiO and the $X\,^2\Sigma^+$ and $A\,^2\Pi$ states of SiO^+ 73 (1982) 169
Wickham-Jones, C.T., see M.M. Maricq 75 (1983) 347
Wickramaaratchi, M.A., see A.S. Manocha 76 (1983) 129
Wiersma, D.A., see J.B.W. Morsink 71 (1982) 289
Wikander, G. and O.E. Mogensen, A study of picosecond dehalogenation of chlorobenzene anions in liquids by positronium inhibition measurements 72 (1982) 407
Wikander, G., O.E. Mogensen and N.-J. Pedersen, Inhibition of Ps formation in benzene and cyclohexane by CH_3Cl and CH_3Br. Correlation to radiation chemistry results 77 (1983) 159
Wild, U.P., see G.W. Suter 73 (1982) 421
Wildt, J., E.H. Fink, R. Winter and F. Zabel, Radiative lifetime and quenching of $SO(b\,^1\Sigma^+, v' = 0)$ 80 (1983) 167
Wilhelm, J., see M. Capitelli 79 (1983) 1
Willems, P., H. Hulsman and F. Aerts, On the use of laser-induced fluorescence to study free-jet expansions 71 (1982) 27
Willoughby, L.C., see A.C. Legon 74 (1983) 127
Winkler, R., see M. Capitelli 79 (1983) 1
Winnewisser, M. and E.W. Peau, The vibrational energy manifold of the lowest lying bending mode of tricarbon oxide sulfide, O=C=C=C=S, as determined by relative intensity measurements 71 (1982) 377

Winscom, C.J., see W. Fröhling 75 (1983) 389
Winter, R., see J. Wildt 80 (1983) 167
Wittig, C., see T.A. Watson 78 (1983) 57
Wolf, H.C., see R. Krauss 73 (1982) 55
Wolf, H.C., see W. Höptner 73 (1982) 253
Woolfe, G.J., M. Melzig, S. Schneider and F. Dörr, The role of tautomeric and rotameric species in the photophysics of 2-(2′-hydroxyphenyl)benzoxazole 77 (1983) 213
Wrigley, S.P., K.W. Smith and B.S. Rabinovitch, Intramolecular vibrational relaxation in the dual-channel 5-methyl-3-hexyl radical system excited by different activation pathways 75 (1983) 453

Yamabe, S., see K. Hirao 80 (1983) 237
Yamaguchi, Y., see Y. Osamura 72 (1982) 131
Yang, M., see Ch. Ottinger 76 (1983) 61
Yarwood, J., see U.P. Agarwal 74 (1983) 35
Yarwood, J., see W.F. Pacynko 78 (1983) 319
Yeager, D.L., see J.T. Golab 78 (1983) 175
Yu, Z.X., P.Y. Lu and R.R. Alfano, Temperature dependence of J-band aggregate of the dye 1,1′-diethyl-2,2′-cyanine bromide studied by steady-state and time-resolved picosecond fluorescence spectroscopy 79 (1983) 289

Zabel, F., see J. Wildt 80 (1983) 167
Zambach, W., see D. Klapstein 72 (1982) 101
Zambach, W., see D. Klapstein 77 (1983) 463
Zaskul'nikov, V.M., see V.A. Bagryansky 78 (1983) 41
Zboiński, Z., Are new chemical species in anthracene crystals formed as a result of charge-carrier trapping at physical defects? 75 (1983) 297
Zen, M., see D. Bassi 71 (1982) 239
Zewail, A.H., see D.P. Millar 72 (1982) 381
Zgierski, M.Z., see W. Siebrand 77 (1983) 35
Zimmerer, G., see Th. Moeller 76 (1983) 295
Zmbov, K.F., see A. Neubert 76 (1983) 469
Zülicke, L., see F. Schneider 76 (1983) 259
Zürcher, H.U., U. Brühlmann and J.R. Huber, Photochemical decay of butanyl ($H_3CC{\equiv}C{-}CHO$) in the gas phase following $S_1(n\pi^*) \leftarrow S_0$ excitation 73 (1982) 403
Zusman, L.D., The theory of transitions between electronic states. Application to radiationless transitions in polar solvents 80 (1983) 29
Zyss, J., see I. Ledoux 73 (1982) 203

SUBJECT INDEX TO VOLUMES 71–80

METHODS

Theoretical

Group theory and algebras

Superfine and hyperfine structure in the ν_3 band of $^{32}SF_6$, J. Bordé and Ch.J. Bordé 71 (1982) 417
The polarization dependence of two-photon absorption rates for randomly oriented molecules, M.A.C. Nascimento 74 (1983) 51
Time-reversal symmetry, Kramers' degeneracy and the algebraic eigenvalue problem, N. Rösch 80 (1983) 1

Classical mechanics and field theory

Laser-induced ultrasonics: a dynamic holographic approach to the measurement of weak absorptions, optoelastic constants and acoustic attenuation, R.J.D. Miller, R. Casalegno, K.A. Nelson and M.D. Fayer 72 (1982) 371
Electrostatic energy of vacancy formation in crystals of polar molecules, R.W. Munn 74 (1983) 301
Polarization energy of a localized charge in a molecular crystal. IV. Effect of polarizability changes, I. Eisenstein, R.W. Munn and P.J. Bounds 74 (1983) 307
Classical aspects of the laser excitation of a Morse oscillator, S.K. Gray 75 (1983) 67
A model of localization, soliton propagation, and self-trapping in an electronically excited atomic lattice, M.A. Collins and D.P. Craig 75 (1983) 191
The semiclassical determination of potential surfaces from observed spectra. I, S.M. Colwell and I.C. Percival 75 (1983) 215
The semiclassical determination of potential surfaces from observed spectra. II, S.M. Colwell and I.C. Percival 75 (1983) 225
Chaotic motions in vibrating molecular: the generalized Hénon–Heiles, R. Ramaswamy 76 (1983) 15
Unified theory of the electronic Stark effect in molecular crystals, R.W. Munn 76 (1983) 243
The description of molecular large-amplitude motions in terms of curvilinear coordinates associated with the reaction path, A. Nauts and X. Chapuisat 76 (1983) 349
Polarization energy of a localized charge in a molecular crystal. V. Effect of vacancies, I. Einstein and R.W. Munn 77 (1983) 47
Classical trajectory study of the effects of parent-molecule bending and overall rotation in polyatomic direct photofragmentation. Model ICN + $h\nu \rightarrow$ CN + I, M.D. Pattengill 78 (1983) 229
Polarization energy of a localized charge in a molecular crystal. VI. Effect of excitons, I. Eisenstein and R.W. Munn 79 (1983) 189
A new approach to the determination of good action–angle variables for coupled oscillator systems, L.C. Geiger and G.C. Schatz 79 (1983) 431
Classical treatment of a Heisenberg linear chain with spin alternation; application to the MnNi (EDTA)·$6H_2O$ complex, M. Drillon, E. Coronado, D. Beltran and R. Georges 79 (1983) 449

Stationary wavefunctions

Are atoms intrinsic to molecular electronic wavefunctions? I. The FORS model, K. Ruedenberg M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 41

Are atoms intrinsic to molecular electronic wavefunctions? II. Analysis of FORS orbitals, K. Ruedenberg, M.W. Schmidt and M.M. Gilbert 71 (1982) 51
Are atoms intrinsic to molecular electronic wavefunctions? III. Analysis of FORS configurations, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 65
Ab initio calculation of the zero-field splittings of the $X\,^3\Sigma_g^-$ and $B\,^3\Pi_{g,i}$ states of the S_2 molecule, B.A. Hess, R.J. Buenker, C.M. Marian and S.D. Peyerimhoff 71 (1982) 79
Features of the photochemically active state surfaces of azobenzene, S. Monti, G. Orlandi and P. Palmieri 71 (1982) 87
X-ray scattering factors, Compton profiles, and shell corrections from numerical atomic wavefunctions, J. Oddershede and J.R. Sabin 71 (1982) 161
The selection of coordinate systems for describing large-amplitude nuclear motion in triatomic molecules, R. Wallace 71 (1982) 173
The direct reaction field hamiltonian: analysis of the dispersion term and application to the water dimer, B.T. Thole and P.Th. Duijnen 71 (1982) 211
C-13 magnetic relaxation rates and H-1 and C-13 paramagnetic shifts of Ni(II) complex of dopamine, A. Lai, M. Monduzzi, G. Saba, M. Casu and G. Crisponi 71 (1982) 271
On the use of "effective harmonic potentials" and "effective normal coordinates" in computing the vibrational energy levels of polyatomic molecules, G. Amat 71 (1982) 363
α-hydroxyalkyl radicals by photoreduction in aprotic solvents: ESR spectra, ab initio potential function, inversion–internal rotation dynamics and temperature dependence of coupling constants of 1-hydroxyethyl, G. Cirelli, T.-K. Ha, R. Meyer and Hs.H. Günthard 72 (1982) 15
Potential energy curves and transition moments for the low-lying electronic states of the Si_2 molecule, S.D. Peyerimhoff and R.J. Buenker 72 (1982) 111
Atoms-in-molecules calculations on diatomic fragments of polyatomic systems: HeH, HeH^+ and HeH^- for a DIM model of Penning ionization of H_2 by He^*, I. Paidarová, J. Vojtík and R. Polák 72 (1982) 119
Unified theoretical treatment of analytic first and second energy derivatives in open-shell Hartree–Fock theory, Y. Osamura, Y. Yamaguchi, P. Saxe, M.A. Vincent, J.F. Gaw and H.F. Schaefer III 72 (1982) 131
Relativistically parameterized extended Hückel calculations. VII. Nuclear spin–spin coupling tensors and densities of states for cluster models of CdTe, HgTe and PbTe, A. Viste, M. Hotokka, L. Laaksonen and P. Pyykkö 72 (1982) 225
Photoelectron spectra and their relativistic interpretation for gaseous bismuth trihalides, R.G. Egdell, M. Hotokka, L. Laaksonen, P. Pyykkö and J.G. Snijders 72 (1982) 237
The structure of F_2O_2: theoretical predictions and comparisons with F_2 and F_2O, R. Ahlrichs and P.R. Taylor 72 (1982) 287
Theoretical studies of the electronic spectrum of thioformaldehyde, P.G. Burton, S.D. Peyerimhoff and R.J. Buenker 73 (1982) 83
An ab initio molecular orbital study of the ammonium radical, B.N. McMaster, J. Mrozek and V.H. Smith Jr. 73 (1982) 131
Ab initio calculations of radiative transition probabilities in the $X\,^1\Sigma^+$ state of SiO and the $X\,^2\Sigma^+$ and $A\,^2\Pi$ states of SiO^+, H.-J. Werner, P. Rosmus and M. Grimm 73 (1982) 169
The Franck–Condon principle for radiationless transitions in molecules and a selection rule for Morse oscillators, E.S. Medvedev 73 (1982) 243
On the relativistic theory of NMR chemical shifts, P. Pyykkö 74 (1983) 1
Calculation on the ^{14}N and ^2H quadrupole coupling tensor in trimeric imidazole, M.H. Palmer, F.E. Scott and J.A.S. Smith 74 (1983) 9
Limited configuration interaction calculation of the optical spectrum for the permanganate ion, H. Johansen and S. Rettrup 74 (1983) 77

A model for two-electron four-center mixed valence systems. Application to $[W_4O_8Cl_8(H_2O)_4]^{2-}$, J.J. Girerd and J.P. Launay 74 (1983) 217
Spectroscopic properties of the methyl radical calculated from UHF SCEP wavefunctions, P. Botschwina, J. Flesch and W. Meyer 74 (1983) 321
Large-amplitude vibration in triatoms. II. Introduction of potential refinement within a LAV model applied to the sulfur dioxide molecule, R. Wallace 74 (1983) 339
Semi-empirical corrections to the mixing coefficients for the diatomics-in-molecules method, P.J. Kuntz and C.C. Chang 75 (1983) 79
Electronic structure of potassium clusters (K_9, K_{15}, K_{27}) by the SCF Xα(LSD) SW method, A. Pellegatti, B.N. McMaster and D.R. Salahub 75 (1983) 83
The semiclassical determination of potential surfaces from observed spectra. I, S.M. Colwell and I.C. Percival 75 (1983) 215
The semiclassical determination of potential surfaces from observed spectra. II, S.M. Colwell and I.C. Percival 75 (1983) 225
A combination of pseudopotentials and density functionals: results for Li_n^{m+}, Na_n^{m+} and K_n^{m+} clusters ($n \leqslant 4$; $m = 0,1$), J. Flad, G. Igel, M. Dolg, H. Stoll and H. Preuss 75 (1983) 331
A crystal orbital investigation on the one-dimensional bis(glyoximato)pyrazine iron system, M.C. Böhm 76 (1983) 1
The radiative lifetime of the $A\,^1\Pi$ state of CH^+ calculated from long CAS SCF expansions, M. Larsson and P.E.M. Siegbahn 76 (1983) 175
Diatomics-in-molecules potential energy surfaces of $(HeH_2)^+$: an extended basis set calculation, F. Schneider, L. Zülicke, R. Polák and J. Vojtík 76 (1983) 259
Experimental and theoretical study on cation radicals of cyclopropane, cyclobutane and cyclopentane, K. Ohta, H. Nakatsuji, H. Kubodera and T. Shida 76 (1983) 271
Large-amplitude vibration in triatoms. III. Application to linear molecules: vibrational states of HCN, R. Wallace 76 (1983) 421
The N1s shake-up spectrum of para-aminobenzonitrile. A theoretical and experimental ESCA study, P.-Å. Malmquist, S. Svensson and H. Ågren 76 (1983) 429
Long-range interactions of Li($n = 2$) states with each other and the long-range interaction of Li($2s\,^2S$) with Li($3s\,^2S$), D.D. Konowalow and J.L. Fish 77 (1983) 435
Structure and properties of a model of deoxyheme. An ab initio SCF calculation, M.-M. Rohmer, A. Dedieu and A. Veillard 77 (1983) 449
Accessibility of the lowest quintet state of organic molecules through triplet–triplet annihilation; an INDO CI study, B. Dick and B. Nickel 78 (1983) 1
Theoretical three-dimensional potential-energy surface for the reaction of Be with HF, S. Chapman, M. Dupuis and S. Green 78 (1983) 93
Atoms-in-molecules study of ground- and excited-state potential-energy curves for Li_2, R. Polák and J. Vojtík 78 (1983) 107
Magnetic field effects of the recombination of radical ions in reaction centers of photosynthetic bacteria, W. Lersch and M.E. Michel-Beyerle 78 (1983) 115
Proper characterization of MC SCF stationary points, J.T. Golab, D.L. Yeager and P. Jørgensen 78 (1983) 175
On the Ne–Ne potential-energy curve and related properties, R.A. Aziz, W.J. Meath and A.R. Allnatt 78 (1983) 295
Hartree–Fock–Slater LCAO calculation of the Mössbauer parameters of some antimony compounds, W. Ravenek, J.W.M. Jacobs and A. van der Avoird 78 (1983) 391
Valence-shell photoabsorption by CO_2 and its connections with electron–CO_2 scattering, P.M. Dittman, D. Dill and J.L. Dehmer 78 (1983) 405

Can the H_5 molecule be observed?, K. Kaufmann, M. Jungen and V. Staemmler 79 (1983) 111
Ab initio studies on hydrogen-bonded chains. III. The linear, infinite chain of hydrogen cyanide molecules, A. Karpfen 79 (1983) 211
Finite perturbation MCSCF and CI calculations of nuclear spin–spin coupling constants for some molecules with multiple bonds, A. Laaksonen, J. Kowalewski and V.R. Saunders 80 (1983) 221
Theoretical study of shake-up in the core photoelectron spectra of the alkali atoms, G. de Alti, P. Decleva and A. Lisini 80 (1983) 229
Theoretical study on the structure and stability of hydrogen-ion clusters H_n^+ and H_n^- (n = 3,5,7,9,11,13), K. Hirao and S. Yamabe 80 (1983) 237

Coupling schemes
Fermi-coupled spherically adapted effective states in the collisionless multiphoton excitation of SF_6, C. di Lauro and F. Lattanzi 71 (1982) 233
On the use of "effective harmonic potentials" and "effective normal coordinates" in computing the vibrational energy levels of polyatomic molecules, G. Amat 71 (1982) 363
Highly resolved optical spectra of *o*-durylene, W.P. Cofino, G.Ph. Hoornweg, C. Gooijer, C. MacLean and N.H. Velthorst 72 (1982) 73
Random coupling models. IV. Numerical investigation of the dependence on the random coupling distribution and on the initial phases, B. Carmeli, R. Tulman, A. Nitzan and M.H. Kalos 72 (1982) 363
Comment on collisionless vibrational relaxation, W. Fuss 76 (1983) 343
Vibronic and multimode effects on the Raman excitation profile of a totally symmetric fundamental in the Soret band of cytochrome **c**, W. Siebrand and M.Z. Zgierski 77 (1983) 35
Classical treatment of a Heisenberg linear chain with spin alternation; application to the MnNi (EDTA)·$6H_2O$ complex, M. Drillon, E. Coronado, D. Beltran and R. Georges 79 (1983) 449

Transport and relaxation theory
The fluctuating-force formulation of friction drag coefficients, J.M. Schurr 71 (1982) 101
Molecular dynamics computer simulation of liquid dichloromethane. I. Equilibrium properties, M. Ferrario and M.W. Evans 72 (1982) 141
Computer simulation of dichloromethane. II. Molecular dynamics, M. Ferrario and M.W. Evans 72 (1982) 147
Vibrational–translational/rotational and vibrational–vibrational processes in methane/inert-gas mixtures: optoacoustic phase measurements, E. Avramides and T.F. Hunter 74 (1983) 25
Vibrational relaxation times in polyatomic gas mixtures: on the validity of the linear mixture rule, Y.V. Chalapati Rao and B.V. Mallu 74 (1983) 43
Non-hydrodynamic contribution to the concentration dependence of the self diffusion of interacting brownian macroparticles, G.D.J. Phillies 74 (1983) 197
Electron hopping and magnetic field dependent spin dynamics of radical ions in solution, H.W. Krüger, M.E. Michel-Beyerle and E.W. Knapp 74 (1983) 205
An efficient solution of weak-collision master equations in thermal unimolecular reaction rate theory, H.W. Schranz and S. Nordholm 74 (1983) 365
Vibrationally excited molecules and mechanisms of chemical and physical processes in non-equilibrium plasmas, P.A. Sergeev and D.I. Slovetsky 75 (1983) 231
On the statistics of an ensemble of oscillators under excitation. IV. Evaluation of the time for kinetic excitation into the quasicontinuum based on Kramers' theory, V.N. Sazonov and I.E. Khromov 76 (1983) 25
Binary theory of dephasing in liquid solutions. I. The non-markovian theory of encounters, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 149

Binary theory of dephasing in liquid solutions. II. Motion-transformed isotropic Raman spectra, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 163
Some problems of recombination kinetics. I, E. Kotomin and V. Kuzovkov 76 (1983) 479
Dependence of photochemical and photophysical hole burning on laser intensity, A.U. Jalmukhambetov and I.S. Osad'ko 77 (1983) 247
Hopping transport and energy transfer in substitutionally disordered media, B. Sipp 77 (1983) 257
Eigenvalues of the Boltzmann collision operator for binary gases: relaxation of anisotropic distributions, B. Shizgal and R. Blackmore 77 (1983) 417
Dynamics of energy transport in ternary molecular solids. II. Time evolution of naphthalene fluorescence, P. Argyrakis and R. Kopelman 78 (1983) 251
Non-Condon scheme of radiationless transitions for the Morse oscillator model, A.L. Sobolewski 78 (1983) 265
Interaction potentials for Li^+–rare-gas systems, L.A. Viehland 78 (1983) 279
Viscosity dependence of internal conversion rates of polyatomic molecules, K.-E. Süsse, D.-G. Welsch and I. Madzgalla 78 (1983) 443
Collision dominated relaxation of electrons in a weakly ionized nitrogen plasma after abrupt change of the electric field, M. Capitelli, C. Gorse, J. Wilhelm and R. Winkler 79 (1983) 1
Dispersive singlet exciton motion in an organic glass, R. Jankowiak and H. Bässler 79 (1983) 57
On the theory of adiabatic electron-transfer reactions in polar solvents, A.B. Helman 79 (1983) 235
Internal heavy-atom effect on the T_1 states of monochloroquinolines and monochloronaphthalenes, J. Najbar, W. Jarzeba and Z.H. Urbanek 78 (1983) 245
Dipole–phonon coupling and dielectric relaxation, R. Nigmatullin and L.A. Dissado 79 (1983) 455
Charge transfer in polar media. Transition-state entropy, Yu.I. Dakhnovskii and A.A. Ovchinnikov 80 (1983) 17
The theory of transitions between electronic states. Application to radiationless transitions in polar solvents, L.D. Zusman 80 (1983) 29
Comment on "Scaling relationships in photoelectron–photoion coincidence studies: the acetone ion dissociation", D.J. McAdoo 80 (1983) 203
Theory of coherence effects in time-dependent delayed fluorescence. II. Application of two- and three-dimensional crystals, A. Fort, V. Ern and V.M. Kenkre 80 (1983) 205

Statistical mechanics of equilibrium and stationary states

Intermolecular energy transfer probabilities of strong colliders, O. Herscovitz, E. Tzidoni and I. Oref 71 (1982) 221
Molecular dynamics computer simulation of liquid dichloromethane. I. Equilibrium properties, M. Ferrario and M.W. Evans 72 (1982) 141
Use of computer simulation to determine the triplet distribution function in dense fluids, S. Gupta, J.M. Haile and W.A. Steele 72 (1982) 425
Computer simulation studies of anisotropic systems. IX. The Maier–Saupe theory for nematic liquid crystals and the molecular field approximation, G.R. Luckhurst, S. Romano and P. Simpson 73 (1982) 337
Chiral discrimination in the liquid state: a hard-core model for the rôle of repulsive forces, D.P. Craig and I.R. Elsum 73 (1982) 349
Resonant non-linear spectroscopy in strong fields, B. Dick and R.M. Hochstrasser 75 (1983) 133
Fractionally charged ions in crystal lattices of organic ion-radical salts, L. Komorowski 76 (1983) 31
Quantum-mechanical spectral moments in collision-induced light scattering and collision-induced absorption in rare gases at low densities, M. Moraldi 78 (1983) 243
Theory of sorption of gases on polymers. II. Effects of inter-chain secondary bonds, M. Pyda and M. Kurzyński 79 (1983) 219

On the dielectric theory and computer simulation of water, O. Steinhauser 79 (1983) 465
Influence of box shape on the hard-disk pressure at high fluid density, W. Schreiner and K.W. Kratky 80 (1983) 245

Thermodynamics and hydrodynamics
Turbulence in fluids and plasmas, D. ter Haar 71 (1982) 345
Molecular interactions and reorientational motion of neat acetone in the liquid state. ^{17}O NMR chemical shifts and linewidths at variable temperature, B. Ancian, B. Tiffon and J.-E. Dubois 74 (1983) 171
The shape of the Lorentz cavity and the internal field in anisotropic fluids, D.A. Dunmur and R.W. Munn 76 (1983) 249
Isothermal–isobaric molecular dynamics, D.J. Evans and G.P. Morriss 77 (1983) 63

Many-body approaches
Near-degeneracy effects and efficiency of MBPT calculations of molecular properties. Polarizability curve of H_2, G.H.F. Diercksen, M. Jaszuński and A.J. Sadlej 71 (1982) 105
Electronic properties by Green's function calculations. Renormalized optical potential results: Ne, Ar, HF, H_2O, NH_3, I. Cacelli, R. Moccia and V. Carravetta 71 (1982) 199
Dynamic polarizability of many-electron systems within a time-dependent density-functional theory, S.K. Ghosh and B.M. Deb 71 (1982) 295
A spin-adapted linear response theory in a coupled-cluster framework for direct calculation of spin-allowed and spin-forbidden transition energies, S. Ghosh, D. Mukherjee and S.N. Bhattacharyya 72 (1982) 161
Ab initio study on cyanamide and isocyanamide, K. Ichikawa, Y. Hamada, Y. Sugawara, M. Tsuboi, S. Kato and K. Morokuma 72 (1982) 301
Theoretical studies of ion neutralization: two-dimensional tight binding models, H.K. McDowell 72 (1982) 451
Van der Waals forces and molecular diffraction from metal surfaces, with application to Ag(111), N.R. Hill, M. Haller and V. Celli 73 (1982) 363
Molecular translational–rovibronic hamiltonian. I. Non-linear molecules, R. Islampour and M. Kasha 74 (1983) 67
Semiclassical theory for atom–surface scattering calculations on Ar + W (110), G.D. Billing 74 (1983) 143
Convergence of an improved CIPSI algorithm, S. Evangelisti, J.-P. Daudey and J.-P. Malrieu 75 (1983) 91
Molecular translational–rovibronic hamiltonian. II. Linear molecules, R. Islampour and M. Kasha 75 (1983) 157
Cluster expansion of the wavefunction. Valence and Rydberg excitations, ionizations, and inner-valence ionizations of CO_2 and N_2O studied by the SAC and SAC CI theories, H. Nakatsuji 75 (1983) 425
Density functional estimates of charge transfer and chemical potentials in hydrogen halides and mixed halides, J.A. Alonso and N.H. March 76 (1983) 121
An extended Hückel study of hydrogen and oxygen chemisorption on Ru(001) surface, B.C. Khanra and S.K. Saha 76 (1983) 255
Cluster expansion of the wavefunction. Outer- and inner-valence ionization spectra of CS_2 and COS, H. Nakatsuji 76 (1983) 283
Double-ionization Auger satellites obtained by the Green's function method, C.-M. Liegener 76 (1983) 397
Some problems of recombination kinetics. I, E. Kotomin and V. Kuzovkov 76 (1983) 479
Perturbation theory of the electron correlation effects for atomic and molecular properties. VI. Complete active space (CAS) SCF and MBPT calculations of electric properties of the FH molecule, G.H.F. Diercksen, V. Kellö, B.O. Roos and A.J. Sadlej 77 (1983) 93

Hopping transport and energy transfer in substitutionally disordered media, B. Sipp 77 (1983) 257
Finite-field many-body perturbation theory. VI. Multipole polarizabilities of beryllium. A comparative study, G.H.F. Diercksen and A.J. Sadlej 77 (1983) 429
Proper characterization of MC SCF stationary points, J.T. Golab, D.L. Yeager and P. Jørgensen 78 (1983) 175
Complete valence-shell ionization spectra of N_2 and CO: application of the extended two-particle–hole Tamm–Dancoff approximation (2ph-TDA), J. Schirmer and O. Walter 78 (1983) 201
Comparisons between experimental argon and Lennard-Jones 12:6 shear viscosities, D. Fincham and D.M. Heyes 78 (1983) 425
EOM/propagator ionization potentials: extension of the excitation operator manifold, J. Baker 79 (1983) 117
Ab initio CI study of the photodissociation of nitrosyl chloride (ClNO), D. Solgadi, F. Lahmani, C. Lardeux and J.P. Flament 79 (1983) 225
Dipole–phonon coupling and dielectric relaxation, R. Nigmatullin and L.A. Dissado 79 (1983) 455
Breakdown in the Koopmans' theorem interpretation of the outer valence-level photoemission spectra of selected organic molecules, R.W. Bigelow 80 (1983) 45

Collective excitations and quasiparticles
The motion of triplet excitons in β-phase crystals of 9,10-dichloroanthracene, R. Krauss, W. Schrof, H.C. Wolf and D. Schmid 73 (1982) 55
Anharmonic processes in molecular crystals. Calculation of the anharmonic shifts, bandwidths and energy decay processes in crystalline naphthalene, R.G. Della Valle, P.F. Fracassi, R. Righini and S. Califano 74 (1983) 179
A model of localization, soliton propagation, and self-trapping in an electronically excited atomic lattice, M.A. Collins and D.P. Craig 75 (1983) 191
Dipole–phonon coupling and dielectric relaxation, R. Nigmatullin and L.A. Dissado 79 (1983) 455
A theoretical estimate for quasihomopolar singlet levels in long polyenes with a spin model hamiltonian, K. Hashimoto 80 (1983) 253

Computational methods
On the use of laser-induced fluorescence to study free-jet expansions, P. Willems, H. Hulsman and F. Aerts 71 (1982) 27
Ab initio calculation of the zero-field splittings of the $X\,^3\Sigma_g^-$ and $B\,^3\Pi_{g,1}$ states of the S_2 molecule, B.A. Hess, R.J. Buenker, C.M. Marian and S.D. Peyerimhoff 71 (1982) 79
The application of exterior complex scaling in calculations on resonances in nuclear motion in molecular systems, J. Turner and C.W. McCurdy 71 (1982) 127
The selection of coordinate systems for describing large-amplitude nuclear motion in triatomic molecules, R. Wallace 71 (1982) 173
The bond nature of alkaline-earth homonuclear metal clusters investigated with pseudopotential CI method, P. Pacchioni and J. Koutecký 71 (1982) 181
Analysis of the steric dependence of the CH_3I + Rb reaction using a Legendre expansion technique, S. Stolte, K.K. Chakravorty, R.B. Bernstein and D.H. Parker 71 (1982) 353
Unified theoretical treatment of analytic first and second energy derivatives in open-shell Hartree–Fock theory, Y. Osamura, Y. Yamaguchi, P. Saxe, M.A. Vincent, J.F. Gaw and H.F. Schaefer III 72 (1982) 131
Computer simulation of dichloromethane. II. Molecular dynamics, M. Ferrario and M.W. Evans 72 (1982) 147
Ab initio calculation of the equilibrium geometry and the ^{13}C, ^{17}O and ^{27}Al NMR chemical shielding tensors of the system Al^{3+}/CO, Th. Weller, W. Meiler, A. Michael, H.J. Köhler, H. Lischka and R. Höller 72 (1982) 155

Studies using the CASSCF wavefunction, P.J. Knowles, G.J. Sexton and N.C. Handy 72 (1982) 337
Calculations on the mechanism of ion polymerization in the formaldehyde crystal, M.V. Basilevsky, G.N. Gerasimov and S.I. Petrochenko 72 (1982) 349
On the connection between incubation and relaxation times in thermal unimolecular reactions, H.O. Pritchard and S.R. Vatsya 72 (1982) 447
Theoretical studies of ion neutralization: two-dimensional tight binding models, H.K. McDowell 72 (1982) 451
Theoretical studies of the electronic spectrum of thioformaldehyde, P.C. Burton, S.D. Peyerimhoff and R.J. Buenker 73 (1982) 83
Ab initio calculations as first step towards the structure of free radicals. I. Geometries and energies of the ethyl analogs $NH_2CH_3^+$ and $CH_2NH_3^+$, L. Bonazzola, N. Leray and Y. Ellinger 73 (1982) 145
On the structure and dynamics of liquid benzene, O. Steinhauser 73 (1982) 155
An ab initio study of relationships between bond lengths and the harmonic and anharmonic cross-coupling constants involving the double bonds in hetero-atom substituted conjugated dienes, C.W. Bock, M. Trachtman and P. George 73 (1982) 179
Concurrence of the $n\nu_3$ and $(n-1)\nu_3 + \nu_2 + \nu_6$ vibrational ladders in the collisionless multiphoton excitation of $^{32}SF_6$, C. di Lauro, F. Lattanzi and G. Sanna 73 (1982) 215
α- and β-phases of oxalic acid, $H_2C_2O_4$: vibrational spectra, normal-coordinate calculations, and intermolecular forces, J. de Villepin, A. Novak and D. Bougeard 73 (1982) 291
Computer simulation studies of anisotropic systems, IX. The Maier–Saupe theory for nematic liquid crystals and the molecular field approximation, G.R. Luckhurst, S. Romano and P. Simpson 73 (1982) 337
Limited configuration interaction calculation of the optical spectrum for the permanganate ion, H. Johansen and S. Rettrup 74 (1983) 77
A theoretical study of the condensation reactions of methyl cation with ammonia, water, hydrogen fluoride and hydrogen sulphide, R.H. Nobes and L. Radom 74 (1983) 163
Spectroscopic properties of the methyl radical calculated from UHF SCEP wavefunctions, P. Botschwina, J. Flesch and W. Meyer 74 (1983) 321
An efficient solution of weak-collision master equations in thermal unimolecular reaction rate theory, H.W. Schranz and S. Nordholm 74 (1983) 365
Theoretical solvent effects on molecular structure and spectroscopic properties through the virtual-charge model. Application to the inverted solvatochromy of benzophenone $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ absorption bands, A. Botrel, F. Corre and A. le Beuze 74 (1983) 383
Classical trajectory study of three-body direct photofragmentation of $Cd(CH_3)_2$. Comparison of sampling methods, M.D. Pattengill 75 (1983) 59
Semi-empirical corrections to the mixing coefficients for the diatomics-in-molecules method, P.J. Kuntz and C.C. Chang 75 (1983) 79
Convergence of an improved CIPSI algorithm, S. Evangelisti, J.-P. Daudey and J.-P. Malrieu 75 (1983) 91
The electronic structure of chalcogen hexahalogenides, G.L. Gutsev and A.P. Klyagina 75 (1983) 243
Unusual low-energy isomers for simple radical cations, M.J. Frisch, K. Raghavachari, J.A. Pople, W.J. Bouma and L. Radom 75 (1983) 323
A combination of pseudopotentials and density functionals: results for Li_n^{m+}, Na_n^{m+} and K_n^{m+} clusters ($n \leqslant 4$; $m = 0,1$), J. Flad, G. Igel, M. Dolg, H. Stoll and H. Preuss 75 (1983) 331
Chaotic motions in vibrating molecules: the generalized Hénon–Heiles model, R. Ramaswamy 76 (1983) 15
Studies of some iron dithiolate complexes by the ESCA, Mössbauer and extended Hückel methods, J. Blomquist, U. Helgeson, B. Folkesson and R. Larsson 76 (1983) 71
MS Xα and LCAO Xα calculations of ionization potentials. A comparison with Koopmans' theorem and accurate calculations, G. de Alti, P. Decleva and A. Lisini 76 (1983) 185

Calculated ro-vibrational fine-structure spectrum and weak-field Zeeman splittings of the O_2Ar van der Waals molecule, J. Tennyson and J. Mettes 76 (1983) 195
New type of rotational basis function for quantum-mechanical molecular collision calculations, D.C. Clary 76 (1983) 331
Study of the dependence of spin–orbit matrix elements on AO basis set composition for inner and valence shells: results for the multiplet splitting of $X\,^3\Sigma^-$ and $C\,^3\Pi$ of SO and $X\,^2\Pi$ in SO^+, R. Klotz, C.M. Marian, S.D. Peyerimhoff, B.A. Hess and R.J. Buenker 76 (1983) 367
Theoretical approach to fluorine substitution in X_2NO and X_2CN free radicals. Comparison between ab initio UHF and RHF + perturbation treatments, V. Barone, F. Lelj, N. Russo, Y. Ellinger and R. Subra 76 (1983) 385
The temperature dependence of the structure of water, P.A. Egelstaff and J.H. Root 76 (1983) 405
Isothermal–isobaric molecular dynamics D.J. Evans and G.P. Morriss 77 (1983) 63
Perturbation theory of the electron correlation effects for atomic and molecular properties. VI. Complete active space (CAS) SCF and MBPT calculations of electric properties of the FH molecule, G.H.F. Diercksen, V. Kellö, B.O. Roos and A.J. Sadlej 77 (1983) 93
Oscillator strengths and lifetimes of the C_2 $A\,^1\Pi_u$–$X\,^1\Sigma_g^+$ Phillips system, E.F. van Dishoeck 77 (1983) 277
Ab initio study of the thermodynamic and kinetic stability of the ammonium radical, H. Cardy, D. Liotard, A. Dargelos and E. Poquet 77 (1983) 287
Monte Carlo calculations on unimolecular reactions, energy transfer, and IR-multiphoton decomposition, J.R. Barker 77 (1983) 301
Accessibility of the lowest quintet state of organic molecules through triplet–triplet annihilation; an INDO CI study, B. Dick and B. Nickel 78 (1983) 1
The mechanism of fluorescence quenching of aromatic compounds by acids: ZDO calculations, S.I. Druzhinin and B.M. Uzhinov 78 (1983) 29
Magnetic field effects on the recombination of radical ions in reaction centers of photosynthetic bacteria, W. Lersch and M.E. Michel-Beyerle 78 (1983) 115
Proper characterization of MC SCF stationary points, J.T. Golab, D.L. Yeager and P. Jørgensen 78 (1983) 175
Hartree–Fock–Slater LCAO calculation of the Mössbauer parameters of some antimony compounds, W. Ravenek, J.W.M. Jacobs and A. van der Avoird 78 (1983) 391
Comparisons between experimental argon and Lennard-Jones 12:6 shear viscosities, D. Fincham and D.M. Heyes 78 (1983) 425
The effect of molecular excitation on crystal packing. 9-cyano- and 9,10-dimethylanthracene as excited guest/host and host/guest pairs, K. Norris, P. Gray, D.P. Craig, C.P. Mallett and B.R. Markey 79 (1983) 9
Shape resonances and the photodissociation cross section of MgH near threshold, S.S. Bhattacharyya and D. Basu 79 (1983) 129
A comparison of quantal and semiclassical perturbed-rotational-state methods in H^+–CO collisions, K. Sakimoto 79 (1983) 137
Breathing-sphere quantum calculations of integral and differential cross sections for vibrational excitation in ion (atom)–diatom collisions, G. Drolshagen and J.P. Toennies 79 (1983) 159
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. II. Calculation of spin–orbit coupling, J. Baiardo and M. Vala 79 (1983) 403
Time-reversal symmetry, Kramers' degeneracy and the algebraic eigenvalue problem, N. Rösch 80 (1983) 1
Effective core potential calculations using frozen orbitals. Applications to transition metals, L.G.M. Pettersson, U. Wahlgren and O. Gropen 80 (1983) 7
Breakdown in the Koopmans' theorem interpretation of the outer valence-level photoemission spectra of selected organic molecules, R.W. Bigelow 80 (1983) 45

Finite perturbation MCSCF and CI calculations of nuclear spin–spin coupling constants for some molecules with multiple bonds, A. Laaksonen, J. Kowalewski and V.R. Saunders 80 (1983) 221

Theory of dynamics and scattering
Exchange reactions of hydrogen halides with hydrogenic atoms, D.C. Clary 71 (1982) 117
The application of exterior complex scaling in calculations on resonances in nuclear motion in molecular systems, J. Turner and C.W. McCurdy 71 (1982) 127
Evaluation of an upper bound of the maximal Lyapunov characteristic number by Monte Carlo integration in the chaotic regions of phase space, S.C. Farantos 71 (1982) 157
X-ray scattering factors, Compton profiles, and shell corrections from numerical atomic wavefunctions, J. Oddershede and J.R. Sabin 71 (1982) 161
A semiclassical model for the vibrational excitation of spherical-top molecules in collisions with ions, T. Ellenbroek and J.P. Toennies 71 (1982) 309
Analysis of the steric dependence of the CH_3I + Rb reaction using a Legendre expansion technique, S. Stolte, K.K. Chakravorty, R.B. Bernstein and D.H. Parker 71 (1982) 353
A new extended diffusion model for rotational motion of symmetric-top molecules in the liquid phase, J. Lascombe, M. Besnard and P. Maraval 72 (1982) 177
Two-photon excitations of bond modes, M.L. Sage and J. Jortner 72 (1982) 249
Raman scattering study of toluene vibrational relaxation in benzene–toluene liquid system, W. Reimschüssel, H. Abramczyk, H. Barańska and A. Łabudzinska 72 (1982) 313
Collision-induced absorption in a He–Ar mixture, A. Raczyński 72 (1982) 321
Theoretical studies of ion neutralization: two-dimensional tight binding models, H.K. McDowell 72 (1982) 451
Vibrational deactivation of CO(v = 1) by p-H_2 and o-H_2, L.L. Poulsen and G.D. Billing 73 (1982) 313
Classical differential cross sections and rotational energy transfer distribution for realistic ion–molecule potentials in the CPST limit, F.E. Budenholzer and C.-C. Lee 73 (1982) 323
X-ray structure and optical properties of silver films prepared by condensation of pre-formed Ag-clusters, W. Vogel, B. Tesche and W. Schulze 74 (1983) 137
Semiclassical theory for atom–surface scattering: calculations on Ar + W(110), G.D. Billing 74 (1983) 143
Quantum-mechanical rearrangement processes: off-shell vibrorotational sudden approximation to the dynamics, E. Ficocelli Varracchio 74 (1983) 153
Large-amplitude vibration in triatoms. II. Introduction of potential refinement within a LAV model applied to the sulfur dioxide molecule, R. Wallace 74 (1983) 339
Quantum vibrational transition probabilities from real classical trajectories: asymmetric diatom–diatom collisions, R.T. Skodje, W.R. Gentry and C.F. Giese 74 (1983) 347
The orientation-averaged rotation-decoupled vibration model for product state distributions in light+heavy–heavy reactions, W. Jakubetz 75 (1983) 45
Classical trajectory study of three-body direct photofragmentation of $Cd(CH_3)_2$. Comparison of sampling methods, M.D. Pattengill 75 (1983) 59
Classical aspects of the laser excitation of a Morse oscillator, S.K. Gray 75 (1983) 67
Semi-empirical corrections to the mixing coefficients for the diatomics-in-molecules method, P.J. Kuntz and C.C. Chang 75 (1983) 79
Trajectory surface-hopping study of the K + O_2 collision: energy transfer in neutral and ionic products, G. Parlant, M. Schröder and S. Goursaud 75 (1983) 175
Experimental and theoretical study of the vibrational relaxation of CO(v = 1) and N_2(v = 1): V–T relaxation by the isotopes of helium, M.M. Maricq, E.A. Gregory, C.T. Wickham-Jones, D.J. Cartwright and C.J.S.M. Simpson 75 (1983) 347

Kinetic energy release distribution in the fragmentation of energy-selected iodopropane ions, W.A. Brand, T. Baer and C.E. Klots 76 (1983) 111
Local normal modes and vibrational adiabatic potentials, N. Agmon 76 (1983) 203
Photodissociation kinematics. II. Laboratory angular distributions of a hydride model system and the kinematic isotope effect, K.-M. Chen and C.-C. Pei 76 (1983) 219
Diatomics-in-molecules potential energy surfaces of $(HeH_2)^+$: an extended basis set calculation, F. Schneider, L. Zülicke, R. Polák and J. Vojtík 76 (1983) 259
Semiclassical calculation of energy transfer in polyatomic molecules. VIII. Theory for atom + non-linear triatom, G.D. Billing 76 (1983) 315
New type of rotational basis function for quantum-mechanical molecular collision calculations, D.C. Clary 76 (1983) 331
Comment on collisionless vibrational relaxation, W. Fuss 76 (1983) 343
The description of molecular large-amplitude motions in terms of curvilinear coordinates associated with the reaction path, A. Nauts and X. Chapuisat 76 (1983) 349
Dynamics of a prototype alkali–hydrogen-halide exchange reaction on an ab initio potential-energy surface, I. NoorBatcha and N. Sathyamurthy 77 (1983) 67
Collinear collisions in a well potential, Ch.G. Schlier 77 (1983) 267
Study of IR multiple-photon absorption (MPA) of CF_3Br, E. Borsella, D. Masci, M. Capitelli and M. Dilonardo 77 (1983) 401
Generalized Landau–Zener formula for non-adiabatic transitions between degenerate states, V.V. Likhansky and G.A. Solodovnikov 77 (1983) 409
He–HF vibrational inelasticity at low and intermediate energies from quantum collision theory, F.A. Gianturco, U.T. Lamanna and G. Petrella 78 (1983) 81
Surface hopping trajectory calculations for electronic rotational and vibrational inelastic collisions for the Na–N_2 system, P. Archirel and P. Habitz 78 (1983) 213
Classical trajectory study of the effects of parent-molecule bending and overall rotation in polyatomic direct photofragmentation. Model ICN + $h\nu \rightarrow$ CN + I, M.D. Pattengill 78 (1983) 229
Semiclassical theory of predissociation induced by rotational (Coriolis) coupling, H. Nakamura 78 (1983) 235
Quantum-mechanical spectral moments in collision-induced light scattering and collision-induced absorption in rare gases at low densities, M. Moraldi 78 (1983) 243
Dynamics of energy transport in ternary molecular solids. II. Time evolution of naphthalene fluorescence, P. Argyrakis and R. Kopelman 78 (1983) 251
Valence-shell photoabsorption by CO_2 and its connections with electron–CO_2 scattering P.M. Dittman, D. Dill and J.L. Dehmer 78 (1983) 405
A comparison of quantal and semiclassical perturbed-rotational-state methods in H^+–CO collisions, K. Sakimoto 79 (1983) 137
Theoretical investigation of rotational rainbows in K + N_2 and K + CO collisions, D. Häusler and R. Schinke 79 (1983) 147
Semiclassical calculation of energy transfer in polyatomic molecules. X. Energy transfer in Ar + SF_6 at 1 eV, G.D. Billing 79 (1983) 179
Prediction and interpretation of collinear reactive scattering resonances by the diagonal corrected vibrational adiabatic hyperspherical model, J. Römelt 79 (1983) 197
Comment on "Scaling relationships in photoelectron–photoion coincidence studies: the acetone ion dissociation", D.J. McAdoo 80 (1983) 203
Semiclassical calculation of energy transfer in polyatomic molecules. IX. Cross sections for M + CO_2 (000) → M + CO_2(*nml*)(M = He and Ar), G.D. Billing and D.C. Clary 80 (1983) 213

Experimental

Magnetic and electric resonance

Theory of optically detected magnetic resonance spectra of radical pairs, A.B. Doktorov, O.A. Anisimov, A.I. Burshtein and Yu.N. Molin 71 (1982) 1
C-13 magnetic relaxation rates and H-1 and C-13 paramagnetic shifts of Ni(II) complex of dopamine, A. Lai, M. Monduzzi, G. Saba, M. Casu and G. Crisponi 71 (1982) 271
Avoided-crossing molecular-beam spectroscopy of CH_3SiF_3, W.L. Meerts and I. Ozier 71 (1982) 401
α-hydroxyalkyl radicals by photoreduction in aprotic solvents: ESR spectra, ab initio potential function, inversion–internal rotation dynamics and temperature dependence of coupling constants of 1-hydroxyethyl, G. Cirelli, T.-K. Ha, R. Meyer and Hs.H. Günthard 72 (1982) 15
Ab initio calculation of the equilibrium geometry and the ^{13}C, ^{17}O and ^{27}Al NMR chemical shielding tensors of the system Al^{3+}/CO, Th. Weller, W. Meiler, A. Michael, H.J. Köhler, H. Lischka and R. Höller 72 (1982) 155
Diamagnetic anisotropy of molecular complexes of 1,3,5-trinitrobenzene with anthracene and carbazole, R. Burzyński and T. Luty 72 (1982) 441
The motion of triplet excitons in β-phase crystals of 9,10-dichloroanthracene, R. Krauss, W. Schrof, H.C. Wolf and D. Schmid 73 (1982) 55
Magnetic resonance experiments on the radical cation salt $(fluoranthenyl)_2^+PF_6^-$. Correlation of proton-NMR, fluorine-NMR and ESR, W. Höptner, M. Mehring, J.U. von Schütz, H.C. Wolf, B.S. Morra, V. Enkelmann and G. Wegner 73 (1982) 253
On the relativistic theory of NMR chemical shifts, P. Pyykkö 74 (1983) 1
Calculation of the ^{14}N and ^{2}H quadrupole coupling tensor in trimeric imidazole, M.H. Palmer, F.E. Scott and J.A.S. Smith 74 (1983) 9
Molecular interactions and reorientational motion of neat acetone in the liquid state. ^{17}O NMR chemical shifts and linewidths at variable temperature, B. Ancian, B. Tiffon and J.-E. Dubois 74 (1983) 171
Electron hopping and magnetic field dependent spin dynamics of radical ions in solution, H.W. Krüger, M.E. Michel-Beyerle and E.W. Knapp 74 (1983) 205
Detection of transient laser magnetic resonance signals in pulsed CO_2 laser irradiation of SF_6/H_2O and SF_6/NO mixtures, J.S. Geiger, D.R. Smith and J.D. Bonnett 74 (1983) 239
Detection and identification of free radicals in the gaseous-phase ozonolysis of ethylene: microreactor–matrix ESR spectroscopy, F.J. Rákóczi, R.-K. Ha and Hs.H. Günthard 74 (1983) 273
Kinetics of methyl radical reaction with methanol at 20–105 K, V.L. Vyazovkin, B.V. Bol'shakov and V.A. Tolkatchev 75 (1983) 11
The ESR spectrum of the C_5F_5 radical, T. Chen (Dschen), F. Graf and Hs.H. Günthard 75 (1983) 165
Analysis of restricted rotation of the acetyl group in *m*- and *p*-nitroacetophenone anion radicals, M. Branca, A. Gamba, C. Oliva and M. Simonetta 75 (1983) 253
Structure and photodecomposition reactions of cations of cyclopentane, cyclohexane, cyclic olefines and dienes in γ-irradiated frozen solutions of CF_3CCl_3. An ESR study, M. Tabata and A. Lund 75 (1983) 379
Measurement of the ^{14}N nuclear quadrupole couplings in the lowest ($n\pi^*$) excited triplet state of pyrazine by ODMR, W. Fröhling, C.J. Winscom and K. Möbius 75 (1983) 389
Experimental and theoretical study on cation radicals of cyclopropane, cyclobutane and cyclopentane, K. Ohta, H. Nakatsuji, H. Kubodera and T. Shida 76 (1983) 271
Theoretical approach to fluorine substitution in X_2NO and X_2CN free radicals. Comparison between ab initio UHF and RHF + perturbation treatments, V. Barone, F. Lelj, N. Russo, Y. Ellinger and R. Subra 76 (1983) 385

Electron spin echo decay kinetics of an ion track in β-irradiated frozen solution of sulfuric acid. Numerical simulation by the Monte Carlo method and experiment, A.M. Raitsimring and V.V. Tregub 77 (1983) 123
Delayed-fluorescence ODMR and EPR studies of triplet excitons in charge-transfer molecular crystals, G. Agostini, C. Corvaja, G. Giacometti and L. Pasimeni 77 (1983) 233
An NMR relaxation study of hydrogen exchange and its deuterium isotope effects in aqueous carboxylic acid solutions, D. Lankhorst, J. Schriever and J.C. Leyte 77 (1983) 319
The kinetics of the retarded reaction of free radicals with oxygen in a methanol glass, V.A. Bagryansky, V.M. Zaskul'nikov and V.A. Tolkatchev 78 (1983) 41
Driven-echo and rotary-echo measurements of the spin coherence in triplet-state benzophenone, R. Gillies and A.M. Ponte Goncalves 78 (1983) 49
Magnetic field effects on the recombination of radical ions in reaction centers of photosynthetic bacteria, W. Lersch and M.E. Michel-Beyerle 78 (1983) 115
Flash photolysis electron spin resonance and CIDEP studies of radicals derived from nitrogen heterocyclics. I. The diazanaphthalenes, S. Basu, K.A. McLauchlan and A.J.D. Ritchie 79 (1983) 95

Microwave spectroscopy
The vibrational energy manifold of the lowest lying bending mode of tricarbon oxide sulfide, O=C=C=C=S, as determined by relative intensity measurements, M. Winnewisser and E.W. Peau 71 (1982) 377
Rotational spectrum and hyperfine structure of the $^2\Sigma$ radicals BaF and BaCl, Ch. Ryzlewicz, H.-U. Schütze-Pahlmann, J. Hoeft and T. Törring 71 (1982) 389
Avoided-crossing molecular-beam spectroscopy of CH_3SiF_3, W.L. Meerts and I. Ozier 71 (1982) 401
The rotational spectrum and molecular properties of a hydrogen-bonded dimer of phosphine and hydrogen fluoride, A.C. Legon and L.C. Willoughby 74 (1983) 127
Electric dipole moments of $(HC^{15}N)_2$ and $HC^{15}NH^{35}Cl$, E.J. Campbell and S.G. Kukolich 76 (1983) 225
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. I. Ferroelectric behaviour, H.A. Kołodziej and S. Sorriso 77 (1983) 341
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. II. Isotopic effect, H.A. Kołodziej and S. Sorriso 78 (1983) 75
Conformational energetics in hydrogen-bonded dimers. The unobserved CO–HF complex, M.A. Benzel and C.E. Dykstra 80 (1983) 273

Infrared and Raman spectroscopy
Conformational interconversions in supersonic jets: matrix IR spectroscopy and model calculations, P. Felder and Hs.H. Günthard 71 (1982) 9
Infrared multiple photon excitation of sulfur hexafluoride in a molecular beam, D. Bassi, A. Boschetti, G. Scoles, M. Scotoni and M. Zen 71 (1982) 239
Spectroscopic analysis of the vibrational distribution in dissociative CO–He RF discharges, S. de Benedictis, R. d'Agostini and F. Cramarossa 71 (1982) 247
Inelastic neutron scattering study of low frequency motions in $[Co(C_5H_5)_2^+]$ and $[Cr(C_6H_6)_2^+]$ intercalated in the $MnPS_3$ layered compound, C. Sourisseau, Y. Mathey and C. Poinsignon 71 (1982) 257
Superfine and hyperfine structure in the ν_3 band of $^{32}SF_6$, J. Bordé and Ch.J. Bordé 71 (1982) 417
A new extended diffusion model for rotational motion of symmetric-top molecules in the liquid phase, J. Lascombe, M. Besnard and P. Maraval 72 (1982) 177
Phonon spectra and structure of crystalline ethylene oxide and ethylene sulphide at 77 K, R. Cataliotti and G. Paliani 72 (1982) 293

Ab initio study on cyanamide and isocyanamide, K. Ichikawa, Y. Hamada, Y. Sugawara, M. Tsuboi, S. Kato and K. Morokuma 72 (1982) 301
Raman scattering study of toluene vibrational relaxation in benzene–toluene liquid system, W. Reimschüssel, H. Abramczyk, H. Barańska and A. Łabudzinska 72 (1982) 313
Interpretation of resonance CARS and Shpolskii spectra with calculated molecular geometries, vibrational frequencies and relative intensities: chrysene in its lowest excited singlet and triplet state, Ch. Jung, A. Lau, H.-J. Weigmann, W. Werncke and M. Pfeiffer 72 (1982) 327
Studies of oriented Langmuir–Blodgett multilayers by infrared linear dichroism, P.-A. Chollet and J. Messier 73 (1982) 235
Raman spectroscopy from a picosecond-lived excited state of methyl orange, L.V. Haley and J.A. Koningstein 73 (1982) 263
Stimulated Raman investigation of CO_2-laser-excited SF_6, P. Esherick, A.J. Grimley and A. Owyoung 73 (1982) 271
Some observations on molecular complexes of carbon monoxide in argon and oxygen matrices, M. Diem, T.-L. Tso and E.K.C. Lee 73 (1982) 283
α- and β-phases of oxalic acid, $H_2C_2O_4$: vibrational spectra, normal-coordinate calculations, and intermolecular forces, J. de Villepin, A. Novak and D. Bougeard 73 (1982) 291
Vibrational relaxation of hydrogen-bonded species in solution. IV. Temperature and concentration dependence of the ν_σ(OH---N) band of phenol–pyridine, U.P. Agarwal, R.S. Green and J. Yarwood 74 (1983) 35
Detection of transient laser magnetic resonance signals in pulsed CO_2 laser irradiation of SF_6/H_2O and SF_6/NO mixtures, J.S. Geiger, D.R. Smith and J.D. Bonnett 74 (1982) 239
Theoretical model for calculations of infrared and Raman band profiles of strong hydrogen bonds in ordered media, F. Fillaux 74 (1983) 395
Calculations in infrared and Raman band profiles of strong hydrogen bonds. OH stretching bands and proton dynamics in crystalline potassium hydrogen carbonate, F. Fillaux 74 (1983) 405
Chemical effects in diffusion and structure of zinc chloride in aqueous solution, A.J. Easteal, P.V. Giaquinta, N.H. March and M.P. Tosi 76 (1983) 125
Vibrational energy disposal in reactions of fluorine atoms with hydrides of groups III, IV and V, A.S. Manocha, D.W. Setser and M.A. Wickramaaratchi 76 (1983) 129
Large-amplitude vibration in triatoms. III. Application to linear molecules: vibrational states of HCN, R. Wallace 76 (1983) 421
Space- and time-resolved resonance-enhanced vibrational Raman spectroscopy from a femtosecond-lived singlet excited state of β-carotene, L.V. Haley and J.A. Koningstein 77 (1983) 1
Resonance Raman scattering and absorption spectroscopy of substituted polyenes, J. Berréhar, C. Lapersonne-Meyer, M. Schott and M. le Postollec 77 (1983) 11
Infrared-induced conformational isomerization of ethylene glycol in a low-temperature argon matrix, H. Takeuchi and M. Tasumi 77 (1983) 21
Raman analysis of SF_6 molecular beams excited by a cw CO_2 laser, G. Luijks, J. Timmerman, S. Stolte and J. Reuss 77 (1983) 169
Fermi resonance and bandshapes in deuterated palmitic acid, P. Piaggio, G. Dellepiane, R. Tubino and L. Piseri 77 (1983) 185
Study of IR multiple-photon absorption (MPA) of CF_3Br, E. Borsella, D. Masci, M. Capitelli and M. Dilonardo 77 (1983) 401
Raman spectroscopic studies on the dynamics of a molecular "probe" (methyl iodide) in hydrocarbon solvents, W.F. Pacynko, J. Yarwood and D.J. Gardiner 78 (1983) 319
Infrared laser photoisomerization of 2-fluoroethanol in argon, W.F. Hoffman III and J.S. Shirk 78 (1983) 331
A quantitative analysis of the ν_s(IR) bands of H-bonds. I. Theory, Y. Marechal 79 (1983) 69

A quantitative analysis of the ν_s(IR) bands of H-bonds. II. Adipic acid crystals, Y. Marechal 79 (1983) 85
Spectroscopic properties of Er^{3+} ions in Li(Er, Gs)P_4O_{12} single crystals – fluorescence, Raman and infrared spectra, Z. Mazurak, J. Hanuza, K. Hermanowicz, B. Jeżowska-Trzebiatowska, D. Schultze and Ch. Waligora 79 (1983) 255
Vibrational predissociation of van der Waals clusters of ethylene, G. Fischer, R.E. Miller and R.O. Watts 80 (1983) 147
Matrix-isolation spectroscopy of Pb_2, H. Sontag, B. Eberle and R. Weber 80 (1983) 279

Visible and ultraviolet spectroscopy
Absorption spectra of volatile aromatic hydrocarbon films in the vacuum ultraviolet region, S. Hino, T. Veszprémi, K. Ohno, H. Inokuchi and K. Seki 71 (1982) 135
Spectroscopic analysis of the vibrational distributions in dissociative CO He RF discharges, S. de Benedictis, R. d'Agostino and F. Cramarossa 71 (1982) 247
Photochemical control of energy transfer in molecular crystals, J.S. Patel and D.M. Hanson 72 (1982) 35
X-ray photoemission and optical spectra of $NiPS_3$, $FePS_3$ and $ZnPS_3$, M. Piacentini, F.S. Khumalo, G. Leveque, C.G. Olson and D.W. Lynch 72 (1982) 61
Highly resolved optical spectra of *o*-durylene, W.P. Cofino, G.Ph. Hoornweg, C. Gooijer, C. MacLean and N.H. Velthorst 72 (1982) 73
Low-temperature vibronic spectra of 1,1′-binaphthyl, M.J. Riley, A.R. Lacey, M.G. Sceats and R.G. Gilbert 72 (1982) 83
Inequivalent methyl CH oscillators in methyl-substituted conjugated compounds as revealed by higher overtone spectra, R. Nakagaki and I. Hanazaki 72 (1982) 93
Emission and laser excitation spectra of rotationally cooled cations in the gas phase: $\tilde{A}\,^2\Pi \leftrightarrow \tilde{X}\,^2\Pi$ band systems of $H(C{\equiv}C)_2X^+$, X = Cl, Br, D. Klapstein, J.P. Maier, L. Misev and W. Zambach 72 (1982) 101
Polymerization of TS-12 diacetylene crystals: crystal structures of monomer and polymer and spectroscopy of reaction intermediates, D. Siegel, H. Sixl, V. Enkelmann and G. Wenz 72 (1982) 201
Studies of magnetic field effects on the intensity and the lifetime of sulfur dioxide luminescence in the gas phase, V.I. Makarov, N.L. Lavrik and N.M. Bazhin 72 (1982) 213
Polarization of CN($B\,^2\Sigma^+ – X\,^2\Sigma^+$) emission produced in the electron-impact dissociation of HCN and DCN, T. Nagata, T. Kondow and K. Kuchitsu 72 (1982) 281
Pulse substructure in passively and synchronously mode-locked cw dye lasers, D.P. Millar and A.H. Zewail 72 (1982) 381
Electronic–vibrational excitations of a hydrogen-bonded molecule in supersonic expansions: 1,4-dihydroxyanthraquinone and its deuterated derivatives, G. Smulevich, A. Amirav, U. Even and J. Jortner 73 (1982) 1
Theoretical studies of the electronic spectrum of thioformaldehyde, P.G. Burton, S.D. Peyerimhoff and R.J. Buenker 73 (1982) 83
Electron impact dissociation of molecular hydrogen and deuterium: isotope effect on the emission cross section of H* and D* (n = 3, 4, 5), M. Higo, S. Kamata and T. Ogawa 73 (1982) 99
Picosecond study of pinacyanol photophysics, J.C. Mialocq 73 (1982) 107
An ab initio molecular orbital study of the ammonium radical, B.N. McMaster, J. Mrozek and V.H. Smith Jr. 73 (1982) 131
Photochemical decay of butynal ($H_3CC{\equiv}C$ -CHO) in the gas phase following $S_1(n\pi^*) \leftarrow S_0$ excitation, H.U. Zürcher, U. Brühlmann and J.R. Huber 73 (1982) 403
High-resolution absorption spectra of diphenylmethylenes, D.J. Graham and T.-S. Lin 73 (1982) 411
The dual phosphorescence of benzophenazine in ethanol, G.W. Suter and U.P. Wild 73 (1982) 421
Limited configuration interaction calculation of the optical spectrum for the permanganate ion, H. Johansen and S. Rettrup 74 (1983) 77

Spectra and emission lifetimes of $H_2CS(\tilde{A}\,^1A_2)$, M. Kawasaki, K. Kasatani, Y. Ogawa and H. Sato 74 (1983) 83
Energy-transfer reactions between $He(2\,^3S)$ and $Ne(^3P_{0,2})$ metastable atoms and PN radicals, H. Obase, M. Tsuji and Y. Nishimura 74 (1983) 89
High-resolution spectroscopy of N_2O^+ in the near ultraviolet using FIBLAS (fast-ion-beam laser spectroscopy), S. Abed, M. Broyer, M. Carré, M.L. Gaillard and M. Larzillière 74 (1983) 97
A model for two-electron four-center mixed valence systems. Application to $[W_4O_8Cl_8(H_2O)_4]^{2-}$, J.J. Girerd and J.P. Launay 74 (1983) 217
Excitation and emission spectra of the $^2A_2'' \leftrightarrow {}^2E_1''$ system of the gas-phase cyclopentadienyl radical, H.H. Nelson, L. Pasternack and J.R. McDonald 74 (1983) 227
Theoretical solvent effects on molecular structure and spectroscopic properties through the virtual-charge model. Application to the inverted solvatochromy of benzophenone $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ absorption bands, A. Botrel, F. Corre and A. le Beuze 74 (1983) 383
Jahn–Teller splitting of the $3s \rightarrow 3p$ transition of sodium isolated in a xenon matrix, H. Hormes and J. Schiller 74 (1983) 433
Anomalous rotational distributions in electronic emission of supersonically cooled H_2O^+ $(\tilde{A}\,^2A_1 \rightarrow \tilde{X}\,^2B_1)$, S. Leutwyler, D. Klapstein and J.P. Maier 74 (1983) 441
Photoabsorption spectrum of radicals produced by a pulsed discharge of trace H_2O in Ar, R.L. Day and L.C. Lee 75 (1983) 17
Charge-transfer transitions in crystalline anthracene and their role in photoconductivity, L. Sebastian, G. Weiser, G. Peter and H. Bässler 75 (1983) 103
Fluorescence from the a ^5P and a ^3P states of matrix-isolated Fe atoms, M.T. McKenzie Jr. and E.R. Nixon 75 (1983) 115
A model for the interpretation of the electronic spectra of the complex ions $M(bpy)_3^{2+}$ (M = Fe, Ru, Os) in D_3 and C_2 sites, J. Ferguson and F. Herren 76 (1983) 45
Luminescent charge transfer of ground-state and metastable B^+ ions, Ch. Ottinger, J. Reichmuth and M. Yang 76 (1983) 61
Unified theory of the electronic Stark effect in molecular crystals, R.W. Munn 76 (1983) 243
Spectroscopic investigation of the electronic structure of the chlorine molecule in the VUV, Th. Moeller, B. Jordan, P. Gürtler, G. Zimmerer, D. Haaks, J. le Calve and M.-C. Castex 76 (1983) 295
Solvent effects on the potential energy surfaces of molecular iodine: a spectroscopic study, M. Geilhaupt and Th. Dorfmüller 76 (1983) 443
Optical activity of oriented molecules. IX. Phenomenological Mueller matrix description of thick samples and of optical elements, A. Schönhofer, H.-G. Kuball and C. Puebla 76 (1983) 453
Resonance Raman scattering and absorption spectroscopy of substituted polyenes, J. Berréhar, C. Lapersonne-Meyer, M. Schott and M. le Postollec 77 (1983) 11
Electronic spectra of jet-cooled azulene, M. Fujii, T. Ebata, N. Mikami and M. Ito 77 (1983) 191
Relaxation and spectroscopy of CaCl in seeded supersonic beams, U. Buck, J. Kesper, H.H. Kuge and D. Otten 77 (1983) 201
The role of tautomeric and rotameric species in the photophysics of 2-(2′-hydroxyphenyl)-benzoxazole, G.J. Woolfe, M. Melzig, S. Schneider and F. Dörr 77 (1983) 213
Dynamics of formation of $CN(B\,^2\Sigma^+)$ fragment from HCN and DCN in an argon afterglow, Y. Ozaki, T. Kondow and K. Kuchitsu 77 (1983) 223
Charge transfer to a solvent state. VIII. Localization of charge during the transition state of the solute: the solute cation localization energy, T.B. Truong 77 (1983) 377
Spectroscopic studies of the photochromism of N-salicylideneaniline mixed crystals and glasses, D. Higelin and H. Sixl 77 (1983) 391
Emission spectra of rotationally cooled dihaloacetylene cations in the gas phase: $\tilde{A}\,^2\Pi_{\Omega,g} \rightarrow \tilde{X}\,^2\Pi_{\Omega,u}$ band systems, D. Klapstein, J.P. Maier and W. Zambach 77 (1983) 463

Phosphorescence and E-type delayed fluorescence from azulene in phenazine host crystals, D. Klemp and B. Nickel 78 (1983) 17
Emission spectra of supersonically cooled methyldiacetylene cations, S. Leutwyler, D. Klapstein and J.P. Maier 78 (1983) 151
Emission spectra of supersonically cooled dimethyldiacetylene cations, D. Klapstein, R. Kuhn, S. Leutwyler and J.P. Maier 78 (1983) 167
Dynamics of energy transport in ternary molecular solids. II. Time evolution of naphthalene fluorescence, P. Argyrakis and R. Kopelman 78 (1983) 251
On the use of X-ray-excited optical luminescence (XEOL) for the analysis of multisite rare-earth systems, P. Tola, A. Retournard, J. Dexpert-Ghys, M. Lemonnier, M. Pagel and J. Goulon 78 (1983) 339
On a site-selective EXAFS experiment using optical emission, J. Goulon, P. Tola, M. Lemonnier and J. Dexpert-Ghys 78 (1983) 347
Triplet-state optical spectra of highly concentrated isotopically mixed crystals of anthracene A-h_{10}:A-d_{10}, D. Rund and H. Port 78 (1983) 357
The B $^2\Sigma^+$–X $^2\Sigma^+$ system of SrF: precise spectroscopic constants from a combined fit of microwave and sub-Doppler optical spectra, W.E. Ernst and J.O. Schröder 78 (1983) 363
Collisional and radiational energy transfer in the system $Na^*(3\,^2P) + Na_2(X\,^1\Sigma^+) \rightarrow Na(3\,^2S) + Na_2^*(A\,^1\Sigma^+)$, P. Arrowsmith, S.H.P. Bly, P.E. Charters, P. Chevrier, J.C. Polanyi and H.H. Telle 79 (1983) 31
Rotational and vibrational distributions of $N_2(C\,^3\Pi_u)$ excited by state-selected $Ar(^3P_2)$ and $Ar(^3P_0)$ metastable atoms, T.D. Nguyen and N. Sadeghi 79 (1983) 41
Dispersive singlet exciton motion in an organic glass, R. Jankowiak and H. Bässler 79 (1983) 57
Internal heavy-atom effect on the T_1 states of monochloroquinolines and monochloronaphthalenes, J. Najbar, W. Jarzeba and Z.H. Urbanek 79 (1983) 245
Spectroscopic properties of Er^{3+} ions in Li(Er, Gs)P_4O_{12} single crystals – fluorescence, Raman and infrared spectra, Z. Mazurak, J. Hanuza, K. Hermanowicz, B. Jeżowska-Trzebiatowska, D. Schultze and Ch. Waligora 79 (1983) 255
Fluorescence lifetime and collisional quenching of the predissociative NO B $^2\Pi(v' = 7)$ state, K. Shibuya and F. Stuhl 79 (1983) 367
Formation of NH (A $^3\Pi$, c $^1\Pi$) by electron-impact dissociation of HN_3, I. Tokue and Y. Ito 79 (1983) 383
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. I. Single-crystal polarized absorption spectrum, J. Baiardo, M. Vala and I. Trabjerg 79 (1983) 391
Rotational perturbation in the CN(B $^2\Sigma^+$–X $^2\Sigma^+$) tail band system. I. Analysis of the $v = 27$ and 30 levels of CN(A $^2\Pi_i$), Y. Ozaki, T. Nagata, K. Suzuki, T. Kondow and K. Kuchitsu 80 (1983) 73
Rotational perturbations in the CN(B $^2\Sigma^+$–X $^2\Sigma^+$) tail band system. II. Identification of the CN($^4\Pi$) state and its vibrational levels, Y. Ozaki, H. Ito, K. Suzuki, T. Kondow and K. Kuchitsu 80 (1983) 85
On the role of the dynamic Jahn–Teller effect in the spectra of matrix-isolated atoms with strong spin–orbit coupling, C.M. Weinert, F. Forstmann, R. Grinter and D.M. Kolb 80 (1983) 95
Photofragmentation of HI in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 80 (1983) 113
New I_2 emission from iodine atom recombination reaction, K.-H. Stephan-Rossbach and F.J. Comes 80 (1983) 121
Electronic spectroscopy of fluorobenzene van der Waals molecules by resonant two-photon ionization, K. Rademann, B. Brutschy and H. Baumgärtel 80 (1983) 129
The effect of a magnetic field on discrete and continuum CS_2 fluorescence, S.J. Silvers, M.R. McKeever and G.K. Chawla 80 (1983) 177

Matrix-isolation spectroscopy of Pb_2, H. Sontag, B. Eberle and R. Weber 80 (1983) 279
Singlet exciton migration in a random organic two-component system containing physical and chemical traps, G. Peter, B. Ries and H. Bässler 80 (1983) 289
Determination of the dipole moment of thioformaldehyde in the $\tilde{a}\ ^3A_2$ excited state by laser phosphorescence excitation spectroscopy, D.J. Clouthier and C.M.L. Kerr 80 (1983) 299
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. III. Single-crystal Zeeman spectroscopy, J. Baiardo, M. Vala and I. Trabjerg 80 (1983) 305
On the nature of the fluorescent state of methylated indole derivatives, S.R. Meech, D. Phillips and A.G. Lee 80 (1983) 317
Autoionization spectra of Li_2 and the $X\ ^2\Sigma_g^+$ ground state of Li_2^+: experimental and theoretical investigations, D. Eisel, W. Demtröder, W. Müller and P. Botschwina 80 (1983) 329
Determination of rate constants for some reactions of CBr radicals by VUV laser flash photolysis, L. Hellner, K.T.V. Grattan and M.H.R. Hutchinson 80 (1983) 345
Dissociative excitation of SiH_4, SiD_4, Si_2H_6 and GeH_4 by 0–100 eV electron impact, J. Perrin and J.F.M. Aarts 80 (1983) 351

Photoelectron and ESCA spectroscopy
Synchrotron-radiation photoemission study of the V–VI layered compounds Bi_2Te_3, Bi_2Se_3, Sb_2Te_3 and Sb_2Te_2Se, M.R. Thuler, R.L. Benbow and Z. Hurych 71 (1982) 265
X-ray photoemission and optical spectra of $NiPS_3$, $FePS_3$ and $ZnPS_3$, M. Piacentini, F.S. Khumalo, G. Leveque, C.G. Olson and D.W. Lynch 72 (1982) 61
Photoelectron spectra and their relativistic interpretation for gaseous bismuth trihalides, R.G. Egdell, M. Hotokka, L. Laaksonen, P. Pyykkö and J.G. Snijders 72 (1982) 237
Unimolecular dissociation of excited $C_3H_6O^+$: a comparative photoelectron–photoion coincidence study of 1,2-epoxypropane and acetone, R. Bombach, J.-P. Stadelmann and J. Vogt 72 (1982) 259
Intense shake-up satellites in the XPS spectra of planar and sterically hindered N-piperidyl-nitrobenzenes and -nitrothiophens, G. Distefano, M. Guerra, F.P. Colonna, D. Jones, G. Consiglio and D. Spinelli 72 (1982) 267
Satellites in the X-ray photoelectron spectra of transition-metal and rare-earth compounds, D.D. Sarma, P. Vishnu Kamath and C.N.R. Rao 73 (1982) 71
Autoionization in HCl and DCl by photoelectron spectroscopy, P. Natalis, P. Pennetreau, L. Longton and J.E. Collin 73 (1982) 191
Photoelectron spectroscopic study of simple hydrogen-bonded dimers. I. Supersonic nozzle beam photoelectron spectrometer and the formic-acid dimer, S. Tomoda, Y. Achiba, K. Nomoto, K. Sato and K. Kimura 74 (1983) 113
Photoelectron spectroscopic study of simple hydrogen-bonded dimers. II. The methanol dimer, S. Tomoda and K. Kimura 74 (1983) 121
Angle-resolved photoelectron measurements on the 2p orbitals of Si in SiF_4 and $Si(CH_3)_4$ in the gas phase, P.R. Keller, J.W. Taylor, F.A. Grimm, P. Senn, T.A. Carlson and M.O. Krause 74 (1983) 247
Benchmark measurement of iodobenzene ion fragmentation rates, J. Dannacher, H.M. Rosenstock, R. Buff, A.C. Parr, R.L. Stockbauer, R. Bombach and J.-P. Stadelmann 75 (1983) 23
High-resolution HeI and HeII photoelectron spectra of the zinc and cadmium dihalide valence bands, D.J. Bristow, G.M. Bancroft and J.S. Tse 75 (1983) 263
High-resolution HeI and HeII photoelectron spectra of the Zn 3d and Cd 4d orbitals in the zinc and cadmium dihalides: ligand field splittings and intensity variations, G.M. Bancroft, D.J. Bristow and J.S. Tse 75 (1983) 277

Molecular structure and photoelectron spectra of H_2S, H_2Se, and H_2Te. Effective core potential calculations on ground and valence ionic states, J. Müller, L.J. Sæthre and O. Gropen 75 (1983) 395
Studies of some iron dithiolate complexes by the ESCA, Mössbauer and extended Hückel methods, J. Blomquist, U. Helgeson, B. Folkesson and R. Larsson 76 (1983) 71
Ionization potentials and polarization energies of tetraselenafulvalene (TSF) derivatives determined from ultraviolet photoelectron spectroscopy, N. Sato, G. Saito and H. Inokuchi 76 (1983) 79
The N 1s shake-up spectrum of para-aminobenzonitrile. A theoretical and experimental ESCA study, P.-Å. Malmquist, S. Svensson and H. Ågren 76 (1983) 429
A XANES study of mixed-valence transition-metal oxides and rare-earth alloys, G. Sankar, P.R. Sarode and C.N.R. Rao 76 (1983) 435
Ultrafast non-radiative decay via conical intersections of molecular potential-energy surfaces: $C_2H_4^+$, H. Köppel 77 (1983) 359
Charge transfer to a solvent state. VIII. Localization of charge during the transition state of the solute: the solute cation localization energy, T.B. Truong 77 (1983) 377
High-resolution UV photoelectron spectrum of CO_2, I. Reineck, C. Nohre, R. Maripuu, P. Lodin, S.H. Al-Shamma, H. Veenhuizen, L. Karlsson and K. Siegbahn 78 (1983) 311
Angle-resolved photoelectron spectroscopy of the chloro-substituted methanes, P.R. Keller, J.W. Taylor, T.A. Carlson and F.A. Grimm 79 (1983) 269
Comparison of photon-stimulated dissociation of gas-phase, solid and chemisorbed water, D.E. Ramaker 80 (1983) 183
Angular distribution for the major photoelectron bands of nitrogen below 45 eV binding energy, F.A. Grimm and Th.A. Carlson 80 (1983) 389

Double resonance spectroscopy
Stimulated Raman investigation of CO_2-laser-excited SF_6, P. Esherick, A.J. Grimley and A. Owyoung 73 (1982) 271
Delayed-fluorescence ODMR and EPR studies of triplet excitons in charge-transfer molecular crystals, G. Agostini, C. Corvaja, G. Giacometti and L. Pasimeni 77 (1983) 233
Autoionization spectra of Li_2 and the $X\,^2\Sigma_g^+$ ground state of Li_2^+: experimental and theoretical investigations, D. Eisel, W. Demtröder, W. Müller and P. Botschwina 80 (1983) 329

Lasers
Photon echoes stimulated from long-lived ordered populations in multi-level systems. The effect of intersystem crossing and optical branching, J.B.W. Morsink, W.H. Hesselink and D.A. Wiersma 71 (1982) 289
Photochemical control of energy transfer in molecular crystals, J.S. Patel and D.M. Hanson 72 (1982) 35
Multiphoton dissociation of some volatile uranyl complexes. I. The phenomena of reversible and permanent dissociation, J.E. Eberhardt, I.E. Hoare, D.A. Johnson, R.B. Knott, A.W. Pryor and A.B. Waugh 72 (1982) 41
Multiphoton dissociation of some volatile uranyl complexes. II. Frequency and isotopic effects, J.E. Eberhardt, R.B. Knott and A.W. Pryor 72 (1982) 51
Laser-induced ultrasonics: a dynamic holographic approach to the measurement of weak absorptions, optoelastic constants and acoustic attenuation, R.J.D. Miller, R. Casalegno, K.A. Nelson and M.D. Fayer 72 (1982) 371
Pulse substructure in passively and synchronously mode-locked cw dye lasers, D.P. Millar and A.H. Zewail 72 (1982) 381
Temperature dependence of the reactions of CH radicals with unsaturated hydrocarbons, M.R. Berman, J.W. Fleming, A.B. Harvey and M.C. Lin 73 (1982) 27

Photon-induced molecular charge separation studied by nanosecond time-resolved microwave conductivity, M.P. de Haas and J.M. Warman 73 (1982) 35
Influence of the molecular environment in solution measurements of the second-order optical susceptibility for urea and derivatives, I. Ledoux and J. Zyss 73 (1982) 203
Concurrence of the $n\nu_3$ and $(n-1)\nu_3 + \nu_2 + \nu_6$ vibrational ladders in the collisionless multiphoton excitation of $^{32}SF_6$, C. di Lauro, F. Lattanzi and G. Sanna 73 (1982) 215
Temperature dependence of $C_3(X\,^1\Sigma_g^+)$ reactions with alkenes and alkynes, 295–610 K, H.H. Nelson, H. Helvajian, L. Pasternack and J.R. McDonald 73 (1982) 431
Photofragmentation of H_2S in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 74 (1983) 261
Two-frequency CO_2 laser multiple-photon dissociation and dynamics of excited state absorption in CDF_3, I.P. Herman 75 (1983) 121
Nickel porphyrin photophysics and photochemistry. A picosecond investigation of ligand binding and release in the excited state, D. Kim, C. Kirmaier and D. Holten 75 (1983) 305
Two-photon ionization and dissociation of liquid water by powerful laser UV radiation, D.N. Nikogosyan, A.A. Oraevsky and V.I. Rupasov 77 (1983) 131
Raman analysis of SF_6 molecular beams excited by a cw CO_2 laser, G. Luijks, J. Timmerman, S. Stolte and J. Reuss 77 (1983) 169
Electronic spectra of jet-cooled azulene, M. Fujii, T. Ebata, N. Mikami and M. Ito 77 (1983) 191
The determination of thermal conductivity coefficients of liquids by a thermal lens technique, R.T. Bailey, F.R. Cruickshank, D. Pugh, S. Guthrie, A. McLeod, W.S. Foulds, W.R. Lee and S. Venkatesh 77 (1983) 243
Dependence of photochemical and photophysical hole burning on laser intensity, A.U. Jalmukhambetov and I.S. Osad'ko 77 (1983) 247
The nascent translational energy of difluorocarbene produced in IR MPD of the penta-fluoroethyl radical, D.M. Rayner, S. Kimel and P.A. Hackett 77 (1983) 349
Study of IR multiple-photon absorption (MPA) of CF_3Br, E. Borsella, D. Masci, M. Capitelli and M. Dilonardo 77 (1983) 401
Photolytic production of $O(^3P)$ in the presence of CF_3I: the formation of $IF(X\,^1\Sigma^+)$, T.A. Watson, M. Addison and C. Wittig 78 (1983) 57
Photodissociation of molecular beams of N_2O_4, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 78 (1983) 65
Separation of deuterium by IR multiphoton decomposition of chlorodifluoromethane. IR multiphoton absorption by and decomposition of a CF_2DCl/CF_2HCl mixture, K.O. Kutschke, M. Gauthier and P.A. Hackett 78 (1983) 323
Infrared laser photoisomerization of 2-fluoroethanol in argon, W.F. Hoffman III and J.S. Shirk 78 (1983) 331
Rotational and vibrational distributions of $N_2(C\,^3\Pi_u)$ excited by state-selected Ar $(^3P_2)$ and Ar $(^3P_0)$ metastable atoms, T.D. Nguyen and N. Sadeghi 79 (1983) 41
Deuterium separation and infrared photochemistry in CF_2HCl, J. Moser, P. Morand, R. Duperrex and H. van den Bergh 79 (1983) 277
Argon ion laser excitation of supersonic seeded molecular beams of I_2, F.J. Aoiz, M.M. Oprysko and R.B. Bernstein 79 (1983) 321
Search for the laser-induced crossed beam reaction of excited I_2 $(B\,^2\Pi)$ with Hg, M.M. Oprysko, F.J. Aoiz, R.B. Bernstein and M.A. McMahan 79 (1983) 341
Kinetics and detection of F (^2P) atoms in a discharge flow system, M.A.A. Clyne and A. Hodgson 79 (1983) 351
Band-state interpretation of lattice thermal conductivity and microhardness of ternary chalcopyrite semiconductors, L.K. Samanta, D.K. Ghosh and G.C. Bhar 79 (1983) 361

Fluorescence lifetime and collisional quenching of the predissociative NO B $^2\Pi$ ($v' = 7$) state, K. Shibuya and F. Stuhl 79 (1983) 367
Radiative lifetime and quenching of SO(b $^1\Sigma^+$, $v' = 0$), J. Wildt, E.H. Fink, R. Winter and F. Zabel 80 (1983) 167
Determination of rate constants for some reactions of CBr radicals by VUV laser flash photolysis, L. Hellner, K.T.V. Grattan and M.H.R. Hutchinson 80 (1983) 345
Infrared-enhanced multiphoton dissociation of iodobenzene cations, N.B. Lev and R.C. Dunbar 80 (1983) 367
Intensity dependence of CO_2-laser-induced multiphoton absorption and decomposition of monomethylamine, D.K. Evans, R.D. McAlpine, H.M. Adams and A.L. Creagh 80 (1983) 379

Polarized light
Polarization of CN(B $^2\Sigma^+$–X $^2\Sigma^+$) emission produced in the electron-impact dissociation of HCN and DCN, T. Nagata, T. Kondow and K. Kuchitsu 72 (1982) 281
Phonon spectra and structure of crystalline ethylene oxide and ethylene sulphide at 77 K, R. Cataliotti and G. Paliani 72 (1982) 293
The polarization dependence of two-photon absorption rates for randomly oriented molecules, M.A.C. Nascimento 74 (1983) 51
A model for two-electron four-center mixed valence systems. Application to $[W_4O_8Cl_8(H_2O)_4]^{2-}$, J.J. Girerd and J.P. Launay 74 (1983) 217
Jahn–Teller splitting of the 3s → 3p transition of sodium isolated in a xenon matrix, J. Hormes and J. Schiller 74 (1983) 433
Resonance Rayleigh light scattering of some porphyrins in solution: intensities and depolarization ratios, J. Anglister and I.Z. Steinberg 75 (1983) 443
Optical activity of oriented molecules. IX. Phenomenological Mueller matrix description of thick samples and of optical elements, A. Schönhofer, H.-G. Kuball and C. Puebla 76 (1983) 453
Measurements of depolarization ratios of gaseous linear chain molecules: a test of the principle of the additivity of bond polarizabilities, J.E.M. Haverkort, F. Baas and J.J.M. Beenakker 79 (1983) 105
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. I. Single-crystal polarized absorption spectrum, J. Baiardo, M. Vala and I. Trabjerg 79 (1983) 391
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. III. Single-crystal Zeeman spectroscopy, J. Baiardo, M. Vala and I. Trabjerg 80 (1983) 305

Atomic and molecular beams
Conformational interconversions in supersonic jets: matrix IR spectroscopy and model calculations, P. Felder and Hs.H. Günthard 71 (1982) 9
On the use of laser-induced fluorescence to study free-jet expansions, P. Willems, H. Hulsman and F. Aerts 71 (1982) 27
Exchange reactions of hydrogen halides with hydrogenic atoms, D.C. Clary 71 (1982) 117
Infrared multiple photon excitation of sulfur hexafluoride in a molecular beam, D. Bassi, A. Boschetti, G. Scoles, M. Scotoni and M. Zen 71 (1982) 239
Analysis of the steric dependence of the CH_3I + Rb reaction using a Legendre expansion technique, S. Stolte, K.K. Chakravorty, R.B. Bernstein and D.H. Parker 71 (1982) 353
Emission and laser excitation spectra of rotationally cooled cations in the gas phase: $\tilde{A}\,^2\Pi \leftrightarrow \tilde{X}\,^2\Pi$ band systems of H–(C≡C)$_2$–X$^+$, X = Cl, Br, D. Klapstein, J.P. Maier, L. Misev and W. Zambach 72 (1982) 101
Evidence for the existence of structures in gas-phase homomolecular clusters of water, V. Hermann, B.D. Kay and A.W. Castleman Jr. 72 (1982) 185

Glory undulations in the total cross section of Ar–Ar,Kr,Xe and Kr–Ar,Kr, H.C.W. Beijerinck, P.M.A. van der Kam and N.F. Verster 72 (1982) 391
Microphone detection of pulsed atomic and molecular beams, J.G. Choi and G.J. Diebold 73 (1982) 19
Photodissociation of molecular beams of SO_2 at 193 nm, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 73 (1982) 377
High-resolution spectroscopy of N_2O^+ in the near ultraviolet using FIBLAS (fast-ion-beam laser spectroscopy), S. Abed, M. Broyer, M. Carré, M.L. Gaillard and M. Larzillière 74 (1983) 97
Photofragmentation of H_2S in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 74 (1983) 261
Anomalous rotational distributions in electronic emission of supersonically cooled H_2O^+ ($\tilde{A}\,^2A_1 \rightarrow \tilde{X}\,^2B_1$), S. Leutwyler, D. Klapstein and J.P. Maier 74 (1983) 441
Electronic structure of potassium clusters (K_9, K_{15}, K_{27}) by the SCF Xα(LSD) SW method, A. Pellegatti, B.N. McMaster and D.R. Salahub 75 (1983) 83
Internal energy dependence of the autodetachment and dissociation times of the SF_6^- ion, J.P. Astruc, R. Barbé, A. Lagrèze and J.P. Schermann 75 (1983) 405
Luminescent charge transfer of ground-state and metastable B^+ ions, Ch. Ottinger, J. Reichmuth and M. Yang 76 (1983) 61
Dynamics of a prototype alkali–hydrogen-halide exchange reaction on an ab initio potential-energy surface, I. NoorBatcha and N. Sathyamurthy 77 (1983) 67
Raman analysis of SF_6 molecular beams excited by a cw CO_2 laser, G. Luijks, J. Timmerman, S. Stolte and J. Reuss 77 (1983) 169
Electronic spectra of jet-cooled azulene, M. Fujii, T. Ebata, N. Mikami and M. Ito 77 (1983) 191
Relaxation and spectroscopy of CaCl in seeded supersonic beams, U. Buck, J. Kesper, H.H. Kuge and D. Otten 77 (1983) 201
Emission spectra of rotationally cooled dihaloacetylene cations in the gas phase: $\tilde{A}\,^2\Pi_{\Omega,g} \rightarrow \tilde{X}\,^2\Pi_{\Omega,g}$ band systems, D. Klapstein, J.P. Maier and W. Zambach 77 (1983) 463
Photodissociation of molecular beams of N_2O_4, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 78 (1983) 65
Emission spectra of supersonically cooled methyldiacetylene cations, S. Leutwyler, D. Klapstein and J.P. Maier 78 (1983) 151
Emission spectra of supersonically cooled dimethyldiacetylene cations, D. Klapstein, R. Kuhn, S. Leutwyler and J.P. Maier 78 (1983) 167
State-selected molecular-beam reaction dynamics of K with HF ($v = 1$, $j = 5,6$ and 7), M. Hoffmeister, L. Potthast and H.J. Loesch 78 (1983) 369
Collisional and radiational energy transfer in the system $Na^*(3\,^2P) + Na_2(X\,^1\Sigma^+) \rightarrow Na(3\,^2S) + Na_2^*(A\,^1\Sigma^+)$, P. Arrowsmith, S.H.P. Bly, P.E. Charters, P. Chevrier, J.C. Polanyi and H.H. Telle 79 (1983) 31
Argon ion laser excitation of supersonic seeded molecular beams of I_2, F.J. Aoiz, M.M. Oprysko and R.B. Bernstein 79 (1983) 321
Search for the laser-induced crossed beam reaction of excited I_2 ($B\,^3\Pi$) with Hg, M.M. Oprysko, F.J. Aoiz, R.B. Bernstein and M.A. McMahan 79 (1983) 341
Electronic spectroscopy of fluorobenzene van der Waals molecules by resonant two-photon ionization, K. Rademann, B. Brutschy and H. Baumgärtel 80 (1983) 129
Vibrational predissociation van der Waals clusters of ethylene, G. Fischer, R.E. Miller, and R.O. Watts 80 (1983) 147
Vibrational effects with excitation transfer in metastable rare-gas–halide collisions, M.S. de Vries and R.M. Martin 80 (1983) 157
Autoionization spectra of Li_2 and the $X\,^2\Sigma_g^+$ ground state of Li_2^+: experimental and theoretical investigations, D. Eisel, W. Demtröder, W. Müller and P. Botschwina 80 (1983) 329

Time-resolved experiments
Photon echoes stimulated from long-lived ordered populations in multi-level systems. The effect of intersystem crossing and optical branching, J.B.W. Morsink, W.H. Hesselink and D.A. Wiersma 71 (1982) 289
Time-resolved spectroscopy: wavepacket formalism in the coherent-state representation, A.A. Villaeys and K.F. Freed 72 (1982) 1
Laser-induced ultrasonics: a dynamic holographic approach to the measurement of weak absorptions, optoelastic constants and acoustic attenuation, R.J.D. Miller, R. Casalegno, K.A. Nelson and M.D. Fayer 72 (1982) 371
Pulse substructure in passively and synchronously mode-locked cw dye lasers, D.P. Millar and A.H. Zewail 72 (1982) 381
Temperature dependence of the reactions of CH radicals with unsaturated hydrocarbons, M.R. Berman, J.W. Fleming, A.B. Harvey and M.C. Lin 73 (1982) 27
Photon-induced molecular charge separation studied by nanosecond time-resolved microwave conductivity, M.P. de Haas and J.M. Warman 73 (1982) 35
Picosecond study of pinacyanol photophysics, J.C. Mialocq 73 (1982) 107
Muonium-substituted organic free radicals in liquids. Muon–electron hyperfine coupling constants and the selectivity of formation of methyl- and fluorine-substituted cyclohexadienyl-type radicals, E. Roduner, G.A. Brinkman and P.W.F. Louwrier 73 (1982) 117
Positronium yields in liquids determined by lifetime and angular correlation measurements, O.E. Mogensen and F.M. Jacobsen 73 (1982) 223
Raman spectroscopy from a picosecond-lived excited state of methyl orange, L.V. Haley and J.A. Koningstein 73 (1982) 263
Stimulated Raman investigation of CO_2-laser-excited SF_6, P. Esherick, A.J. Grimley and A. Owyoung 73 (1982) 271
The dual phosphorescence of benzophenazine in ethanol, G.W. Suter and U.P. Wild 73 (1982) 421
Temperature dependence of $C_3(X\,^1\Sigma_g^+)$ reactions with alkenes and alkynes, 295–610 K, H.H. Nelson, H. Helvajian, L. Pasternack and J.R. McDonald 73 (1982) 431
Picosecond kinetics of radiationless relaxations of triphenyl methane dyes. Evidence for rapid excited-state equilibrium between states of differing geometry, V. Sundström, T. Gillbro and H. Bergström 73 (1982) 439
Relaxation of the individual vibrational levels of carbon monoxide following shock heating at 2100 K, J.P. Martin, M.R. Buckingham, J.A. Chenery and C.J.S.M. Simpson 74 (1983) 15
Vibrational–translational/rotational and vibrational vibrational processes in methane/inert-gas mixtures: optoacoustic phase measurements, E. Avramides and T.F. Hunter 74 (1983) 25
Electron hopping and magnetic field dependent spin dynamics of radical ions in solution, H.W. Krüger, M.E. Michel-Beyerle and E.W. Knapp 74 (1983) 205
Vibrational relaxation of CO_2 (00^01) and N_2O (00^01) by NO, F. Al Adel, L. Doyennette, M. Margottin-Maclou and L. Henry 74 (1983) 413
The dipole moment of ^{7}LiH and ^{7}LiD in the excited $A\,^1\Sigma^+$ state: a test of the Born–Oppenheimer approximation, M. Brieger, A. Renn, A. Sodeik and A. Hese 75 (1983) 1
Benchmark measurement of iodobenzene ion fragmentation rates, J. Dannacher, H.M. Rosenstock, R. Buff, A.C. Parr, R.L. Stockbauer, R. Bombach and J.-P. Stadelmann 75 (1983) 23
Are new chemical species in anthracene crystals formed as a result of charge-carrier trapping at physical defects?, Z. Zboiński 75 (1983) 297
Nickel porphyrin photophysics and photochemistry. A picosecond investigation of ligand binding and release in the excited state, D. Kim, C. Kirmaier and D. Holten 75 (1983) 305

Experimental and theoretical study of the vibrational relaxation of CO($v = 1$) and N_2($v = 1$): V–T relaxation by the isotopes of helium, M.M. Maricq, E.A. Gregory, C.T. Wickham-Jones, D.J. Cartwright and C.J.S.M. Simpson 75 (1983) 347
Intramolecular vibrational relaxation in the dual-channel 5-methyl-3-hexyl radical system excited by different activation pathways, S.P. Wrigley, K.W. Smith and B.S. Rabinovitch 75 (1983) 453
Molecular orbital electron momentum distributions and separation energies of CH_3CN, A. Minchinton, C.E. Brion, J.P.D. Cook and E. Weigold 76 (1983) 89
Fluorescence quenching of tertiary amines by halocarbons, P.C. Alford, C.G. Cureton, R.A. Lampert and D. Phillips 76 (1983) 103
Rate constants for vibrational energy transfer between CO ($v = 1$) and CH_4 and substituted methane molecules in the temperature range 300 to 80 K, D.C. Allen and C.J.S.M. Simpson 76 (1983) 231
Space- and time-resolved resonance-enhanced vibrational Raman spectroscopy from a femtosecond-lived singlet excited state of β-carotene, L.V. Haley and J.A. Koningstein 77 (1983) 1
Two-photon ionization and dissociation of liquid water by powerful laser UV radiation, D.N. Nikogosyan, A.A. Oraevsky and V.I. Rupasov 77 (1983) 131
Inhibition of Ps formation in benzene and cyclohexane by CH_3Cl and CH_3Br. Correlation to radiation chemistry results, G. Wikander, O.E. Mogensen and N.-J. Pedersen 77 (1983) 159
The role of tautomeric and rotameric species in the photophysics of 2-(2′-hydroxyphenyl)-benzoxazole, G.J. Woolfe, M. Melzig, S. Schneider and F. Dörr 77 (1983) 213
The determination of thermal conductivity coefficients of liquids by a thermal lens technique, R.T. Bailey, F.R. Cruickshank, D. Pugh, S. Guthrie, A. McLeod, W.S. Foulds, W.R. Lee and S. Venkatesh 77 (1983) 243
The nascent translational energy of difluorocarbene produced in IR MPD of the pentafluoroethyl radical, D.M. Rayner, S. Kimel and P.A. Hackett 77 (1983) 349
Ultrafast non-radiative decay via conical intersections of molecular potential-energy surfaces: $C_2H_4^+$, H. Köppel 77 (1983) 359
Driven-echo and rotary-echo measurements of the spin coherence in triplet-state benzophenone, R. Gillies and A.M. Ponte Goncalves 78 (1983) 49
Photolytic production of O(^{3}P) in the presence of CF_3I: the formation of IF($X\,^1\Sigma^+$), T.A. Watson, M. Addison and C. Wittig 78 (1983) 57
Bifurcation diagrams for two substrate oscillatory systems, J. Maselko 78 (1983) 381
Flash photolysis electron spin resonance and CIDEP studies of radicals derived from nitrogen heterocyclics. I. The diazanaphthalenes, S. Basu, K.A. McLauchlan and A.J.D. Ritchie 79 (1983) 95
Temperature dependence of J-band aggregate of the dye 1,1′-diethyl-2,2′-cyanine bromide studied by steady-state and time-resolved picosecond fluorescence spectroscopy, Z.X. Yu, P.Y. Lu and R.R. Alfano 79 (1983) 289
Vibrational energy relaxation of highly compressed gaseous H_2 and N_2, M. Châtelet, J. Kieffer and B. Oksengorn 79 (1983) 413
Photofragmentation of HI in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 80 (1983) 113
Vibrational effects with excitation transfer in metastable rare-gas–halide collisions, M.S. de Vries and R.M. Martin 80 (1983) 157
Radiative lifetime and quenching of SO ($b\,^1\Sigma^+$, $v' = 0$), J. Wildt, E.H. Fink, R. Winter and F. Zabel 80 (1983) 167
The effect of a magnitude field on discrete and continuum CS_2 fluorescence, S.J. Silvers, M.R. McKeever and G.K. Chawla 80 (1983) 177
Theory of coherence effects in time-dependent delayed fluorescence. II. Application to two- and three-dimensional crystals, A. Fort, V. Ern and V.M. Kenkre 80 (1983) 205

On the nature of the fluorescent state of methylated indole derivatives, S.R. Meech, D. Phillips and A.G. Lee 80 (1983) 317

Cyclotron resonance
Infrared-enhanced multiphoton dissociation of iodobenzene cations, N.B. Lev and R.C. Dunbar 80 (1983) 367

Mass spectra
Electron affinities of higher molybdenum fluorides as determined by the effusion technique, L.N. Sidorov, A.Ya. Borshchevsky, E.B. Rudny and V.D. Butsky 71 (1982) 145
Evidence for the existence of structures in gas-phase homomolecular clusters of water, V. Hermann, B.D. Kay and A.W. Castleman Jr. 72 (1982) 185
Unimolecular dissociations of excited $C_3H_6O^+$: a comparative photoelectron–photoion coincidence study of 1,2-epoxypropane and acetone, R. Bombach, J.-P. Stadelmann and J. Vogt 72 (1982) 259
Dissociation cross sections of silane and disilane by electron impact, J. Perrin, J.P.M. Schmitt, G. de Rösny, B. Drevillon, J. Huc and A. Lloret 73 (1982) 383
Absolute dipole oscillator strengths for molecular and dissociative photoionization of hydrogen fluoride, F. Carnovale and C.E. Brion 74 (1983) 253
The unimolecular dissociation of electronic state-selected methyl iodide cations, I. Powis 74 (1983) 421
Benchmark measurement of iodobenzene ion fragmentation rates, J. Dannacher, H.M. Rosenstock, R. Buff, A.C. Parr, R.L. Stockbauer, R. Bombach and J.-P. Stadelmann 75 (1983) 23
Kinetic energy release distribution in the fragmentation of energy-selected iodopropane ions, W.A. Brand, T. Baer and C.E. Klots 76 (1983) 111
The dissociation energies of gaseous SmLi, EuLi, TmLi and YbLi, A. Neubert and K.F. Zmbov 76 (1983) 469
Kinetic studies of the bromine–oxygen system: a new paramagnetic particle, BrO_2, N.I. Butkovskaya, I.I. Morozov, V.L. Tal'rose and E.S. Vasiliev 79 (1983) 21
Comment on "Scaling relationship in photoelectron–photoion coincidence studies: the acetone ion dissociation", D.J. McAdoo 80 (1983) 203

Radiolysis
A study of picosecond dehalogenation of chlorobenzene anions in liquids by positronium inhibition measurements, G. Wikander and O.E. Mogensen 72 (1982) 407
Positronium yields in liquids determined by lifetime and angular correlation measurements, O.E. Mogensen and F.M. Jacobsen 73 (1982) 223
Reactions induced by ion bombardment of solid cyclohexane at 77 K, O. Puglisi, G. Marletta, S. Pignataro and G. Foti 75 (1983) 417
Inhibition of Ps formation in benzene and cyclohexane by CH_3Cl and CH_3Br. Correlation to radiation chemistry results, G. Wikander, O.E. Mogensen and N.-J. Pedersen 77 (1983) 159

Mössbauer spectroscopy
Studies of some iron dithiolate complexes by the ESCA, Mössbauer and extended Hückel methods, J. Blomquist, U. Helgeson, B. Folkesson and R. Larsson 76 (1983) 71
Mössbauer spectroscopic study of the electronic and magnetic properties of iron(II) para-toluenesulphonate, J.S. Haynes, A.R. Hume, J.R. Sams and R.C. Thompson 78 (1983) 127
Hartree–Fock–Slater LCAO calculation of the Mössbauer parameters of some antimony compounds, W. Ravenek, J.W.M. Jacobs and A. van der Avoird 78 (1983) 391

Diffraction
Polymerization of TS-12 diacetylene crystals: crystal structures of monomer and polymer and spectroscopy of reaction intermediates, D. Siegel, H. Sixl, V. Enkelmann and G. Wenz 72 (1982) 201
X-ray structure and optical properties of silver films prepared by condensation of preformed Ag-clusters, W. Vogel, B. Tesche and W. Schulze 74 (1983) 137
The temperature dependence of the structure of water, P.A. Egelstaff and J.H. Root 76 (1983) 405

P–V–T dependence
Dissociation cross sections of silane and disilane by electron impact, J. Perrin, J.P.M. Schmitt, G. de Rosny, B. Drevillon, J. Huc and A. Lloret 73 (1982) 383
Adiabatic compressibility of critical binary mixtures of nitroethane/isooctane and nitroethane/3-methylpentane, H. Tanaka and Y. Wada 78 (1983) 143
State-selected molecular-beam reaction dynamics of K with HF ($v = 1$, $j = 5,6$ and 7), M. Hoffmeister, L. Potthast and H.J. Loesch 78 (1983) 369
Influence of box shape on the hard-disk pressure at high fluid density, W. Schreiner and K.W. Kratky 80 (1983) 245

Scattering
Inelastic neutron scattering study of low frequency motions in $[Co(C_5H_5)_2^+]$ and $[Cr(C_6H_6)_2^+]$ intercalated in the $MnPS_3$ layered compound, C.Sourisseau, Y. Mathey and C. Poinsignon 71 (1982) 257
State-to-state total cross sections for ion-pair formation, U.C. Klomp and J. Los 71 (1982) 443
Microphone detection of pulsed atomic and molecular beams, J.G. Choi and G.J. Diebold 73 (1982) 19
Influence of the oxy, aza and thio groups on the electron affinities of carbonyl compounds studied by means of ETS, A. Modelli, G. Distefano and D. Jones 73 (1982) 395
Absolute dipole oscillator strengths for molecular and dissociative photoionization of hydrogen fluoride, F. Carnovale and C.E. Brion 74 (1983) 253
Resonance Rayleigh light scattering of some porphyrins in solution: intensities and depolarization ratios, J. Anglister and I.Z. Steinberg 75 (1983) 443
Chemical effects in diffusion and structure of zinc chloride in aqueous solution, A.J. Easteal, P.V. Giaquinta, N.H. March and M.P. Tosi 76 (1983) 125
Neutron scattering study of the reorientational motions in $Cr(CO)_3(\eta^6C_6H_6)$ and $Mn(CO)_3(\eta^5C_5H_5)$, G. Lucazeau, K. Chhor, C. Sourisseau and A.J. Dianoux 76 (1983) 307
Intensities in inelastic neutron scattering spectra: a test of recent theory, J. Howard, B.C. Boland and J. Tomkinson 77 (1983) 145
The nature of the stabilizing effect of thio groups on the Π anion states of benzene studied by means of electron transmission spectroscopy, A. Modelli, D. Jones, F.P. Colonna and G. Distefano 77 (1983) 153
State-selected molecular-beam reaction dynamics of K with HF ($v = 1$, $j = 5,6$ and 7), M. Hoffmeister, L. Potthast and H.J. Loesch 78 (1983) 369
Measurements of depolarization ratios of gaseous linear chain molecules: a test of the principle of the additivity of bond polarizabilities, J.E.M. Haverkort, F. Baas and J.J.M. Beenakker 79 (1983) 105
Quasi-elastic light scattering studies on T7 DNA in the presence of a sinusoidal electric field, K.S. Schmitz 79 (1983) 297

OBJECTS

Bulk systems

Gases

Conformational interconversions in supersonic jets: matrix IR spectroscopy and model calculations, P. Felder and Hs.H. Günthard 71 (1982) 9
On the use of laser-induced fluorescence to study free-jet expansions, P. Willems, H. Hulsman and F. Aerts 71 (1982) 27
Intermolecular energy-transfer probabilities of strong colliders, O. Herscovitz, E. Tzidoni and I. Oref 71 (1982) 221
The vibrational energy manifold of the lowest lying bending mode of tricarbon oxide sulfide, O=C=C=C=S, as determined by relative intensity measurements, M. Winnewisser and E.W. Peau 71 (1982) 377
Multiphoton dissociation of some volatile uranyl complexes. I. The phenomena of reversible and permanent dissociation, J.E. Eberhardt, I.E. Hoare, D.A. Johnson, R.B. Knott, A.W. Pryor and A.B. Waugh 72 (1982) 41
Multiphoton dissociation of some volatile uranyl complexes. II. Frequency and isotopic effects, J.E. Eberhardt, R.B. Knott and A.W. Pryor 72 (1982) 51
Studies of magnetic field effects on the intensity and the lifetime of sulfur dioxide luminescence in the gas phase, C.I. Makarov, N.L. Lavrik and N.M. Bazhin 72 (1982) 213
On the connection between incubation and relaxation times in thermal unimolecular reactions, H.O. Pritchard and S.R. Vatsya 72 (1982) 447
Electron impact dissociation of molecular hydrogen and deuterium: isotope effect on the emission cross section of H^* and D^* ($n = 3, 4, 5$), M. Higo, S. Kamata and T. Ogawa 73 (1982) 99
Concurrence of the $n\nu_3$ and $(n-1)\nu_3 + \nu_2 + \nu_6$ vibrational ladders in the collisionless multiphoton excitation of $^{32}SF_6$, C. di Lauro, F. Lattanzi and G. Sanna 73 (1982) 215
Vibrational deactivation of CO($v = 1$) by p-H_2 and o-H_2, L.L. Poulsen and G.D. Billing 73 (1982) 313
Chiral discrimination in the liquid state: a hard-core model for the rôle of repulsive forces, D.P. Craig and I.R. Elsum 73 (1982) 349
Photodissociation of molecular beams of SO_2 at 193 nm, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 73 (1982) 377
Photochemical decay of butynal ($H_3CO{\equiv}C{-}CHO$) in the gas phase following $S_1(n\pi^*) \leftarrow S_0$ excitation, H.U. Zürcher, U. Brühlmann and J.R. Huber 73 (1982) 403
Relaxation of the individual vibrational levels of carbon monoxide following shock heating at 2100 K, J.P. Martin, M.R. Buckingham, J.A. Chenery and C.J.S.M. Simpson 74 (1983) 15
Vibrational–translational/rotational and vibrational–vibrational processes in methane/inert-gas mixtures: optoacoustic phase measurements, E. Avramides and T.F. Hunter 74 (1983) 25
Vibrational relaxation times in polyatomic gas mixtures: on the validity of the linear mixture rule, Y.V. Chalapati Rao and B.V. Mallu 74 (1983) 43
Spectra and emission lifetime of $H_2CS(\tilde{A}\,^1A_2)$, M. Kawasaki, K. Kasatani, Y. Ogawa and H. Sato 74 (1983) 83
Energy-transfer reactions between $He(2\,^3S)$ and $Ne(^3P_{0,2})$ metastable atoms and PN radicals, H. Obase, M. Tsuji and Y. Nishimura 74 (1983) 89
Angle-resolved photoelectron measurements on the 2p orbitals of Si in SiF_4 and $Si(CH_3)_4$ in the gas phase, P.R. Keller, J.W. Taylor, F.A. Grimm, P. Senn, T.A. Carlson and M.O. Krause 74 (1983) 247
Detection and identification of free radicals in the gaseous-phase ozonolysis of ethylene: microreactor–matrix ESR spectroscopy, F.J. Rákóczi, T.-K. Ha and Hs.H. Günthard 74 (1983) 273

An efficient solution of weak-collision master equations in thermal unimolecular reaction rate theory, H.W. Schranz and S. Nordholm 74 (1983) 365
Vibrational relaxation of CO_2 (00^01) and N_2O(00^01) by NO, F. Al Adel, L. Doyennette, M. Margottin-Maclou and L. Henry 74 (1983) 413
The dipole moment of ^{7}LiH and ^{7}LiD in the excited $A\,^1\Sigma^+$ state: a test of the Born–Oppenheimer approximation, M. Brieger, A. Renn, A. Sodeik and A. Hese 75 (1983) 1
Photoabsorption spectrum of radicals produced by a pulsed discharge of trace H_2O in Ar, R.L. Day and L.C. Lee 75 (1983) 17
The electronic structure of chalcogen hexahalogenides, G.L. Gutsev and A.P. Klyagina 75 (1983) 243
High-resolution HeI and HeII photoelectron spectra of the zinc and cadmium dihalide valence bands, D.J. Bristow, G.M. Bancroft and J.S. Tse 75 (1983) 263
High-resolution HeI and HeII photoelectron spectra of the Zn 3d and Cd 4d orbitals in the zinc and cadmium dihalides: ligand field splittings and intensity variations, G.M. Bancroft, D.J. Bristow and J.S. Tse 75 (1983) 277
Experimental and theoretical study of the vibrational relaxation of CO($v = 1$) and N_2($v = 1$): V–T relaxation by the isotopes of helium, M.M. Maricq, E.A. Gregory, C.T. Wickham-Jones, D.J. Cartwright and C.J.S.M. Simpson 75 (1983) 347
Intramolecular vibrational relaxation in the dual-channel 5-methyl-3-hexyl radical system excited by different activation pathways, S.P. Wrigley, K.W. Smith and B.S. Rabinovitch 75 (1983) 453
On the statistics of an ensemble of oscillators under excitation. IV. Evaluation of the time for kinetic excitation into the quasicontinuum based on Kramers' theory, V.N. Sazonov and I.E. Khromov 76 (1983) 25
Fluorescence quenching of tertiary amines by halocarbons, P.C. Alford, C.G. Cureton, R.A. Lampert and D. Phillips 76 (1983) 103
The radiative lifetime of the $A\,^1\Pi$ state of CH^+ calculated from long CAS SCF expansions, M. Larsson and P.E.M. Siegbahn 76 (1983) 175
Local normal modes and vibrational adiabatic potentials, N. Agmon 76 (1983) 203
Rate constants for vibrational energy transfer between CO ($v = 1$) and CH_4 and substituted methane molecules in the temperature range 300 to 80 K, D.C. Allen and C.J.S.M. Simpson 76 (1983) 231
Semiclassical calculation of energy transfer in polyatomic molecules. VIII. Theory for atom + non-linear triatom, G.D. Billing 76 (1983) 315
The dissociation energies of gaseous SmLi, EuLi, TmLi and YbLi, A. Neubert and K.F. Zmbov 76 (1983) 469
Isothermal–isobaric molecular dynamics, D.J. Evans and G.P. Morriss 77 (1983) 63
The nature of the stabilizing effect of thio groups on the Π anion states of benzene studied by means of electron transmission spectroscopy, A. Modelli, D. Jones, F.P. Colonna and G. Distefano 77 (1983) 153
Dynamics of formation of CN($B\,^2\Sigma^+$) fragment from HCN and DCN in an argon afterglow, Y. Ozaki, T. Kondow and K. Kuchitsu 77 (1983) 223
Monte Carlo calculations on unimolecular reactions, energy transfer, and IR-multiphoton decomposition, J.R. Barker 77 (1983) 301
Study of IR multiple-photon absorption (MPA) of CF_3Br, E. Borsella, D. Masci, M. Capitelli and M. Dilonardo 77 (1983) 401
Eigenvalues of the Boltzmann collision operator for binary gases: relaxation of anisotropic distributions, B. Shizgal and R. Blackmore 77 (1983) 417
Photolytic production of O(^{3}P) in the presence of CF_3I: the formation of IF($X\,^1\Sigma^+$), T.A. Watson, M. Addison and C. Wittig 78 (1983) 57
He–HF vibrational inelasticity at low and intermediate energies from quantum collision theory, F.A. Gianturco, U.T. Lamanna and G. Petrella 78 (1983) 81

Quantum-mechanical spectral moments in collision-induced light scattering and collision-induced absorption in rare gases at low densities, M. Moraldi 78 (1983) 243
Interaction potentials for Li^+–rare-gas systems, L.A. Viehland 78 (1983) 279
Separation of deuterium by IR multiphoton decomposition of chlorodifluoromethane. IR multiphoton absorption by and decomposition of a CF_2DCl/CF_2HCl mixture, K.O. Kutschke, M. Gauthier and P.A. Hackett 78 (1983) 323
Semiclassical calculation of energy transfer in polyatomic molecules. X. Energy transfer in Ar + SF_6 at 1 eV, G.D. Billing 79 (1983) 179
Theory of sorption of gases on polymers. II. Effects of inter-chain secondary bonds, M. Pyda and M. Kurzyński 79 (1983) 219
Deuterium separation and infrared photochemistry in CF_2HCl, J. Moser, P. Morand, R. Duperrex and H. van den Bergh 79 (1983) 277
Kinetics and detection of $F(^2P)$ atoms in a discharge flow system, M.A.A. Clyne and A. Hodgson 79 (1983) 351
Fluorescence lifetime and collisional quenching of the predissociative NO $B\,^2\Pi(v' = 7)$ state, K. Shibuya and F. Stuhl 79 (1983) 367
Formation of NH ($A\,^3\Pi$, $c\,^1\Pi$) by electron-impact dissociation of HN_3, I. Tokue and Y. Ito 79 (1983) 383
Vibrational energy relaxation of highly compressed gaseous H_2 and N_2, M. Châtelet, J. Kieffer and B. Oksengorn 79 (1983) 413
Photofragmentation of HI in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 80 (1983) 113
Comparison of photostimulated dissociation of gas-phase, solid and chemisorbed water, D.E. Ramaker 80 (1983) 183
Semiclassical calculation of energy transfer in polyatomic molecules. IX. Cross sections for $M + CO_2(000) \rightarrow M + CO_2(nml)$(M = He and Ar), G.D. Billing and D.C. Clary 80 (1983) 213
Determination of the dipole moment of thioformaldehyde in the $\tilde{a}\,^3A_2$ excited state by laser phosphorescence excitation spectroscopy, D.J. Clouthier and C.M.L. Kerr 80 (1983) 299
Intensity dependence of CO_2-laser-induced multiphoton absorption and decomposition of monomethylamine, D.K. Evans, R.D. McAlpine, H.M. Adams and A.L. Creagh 80 (1983) 379

Liquids
The fluctuating-force formulation of friction drag coefficients, J.M. Schurr 71 (1982) 101
Turbulence in fluids and plasmas, D. ter Haar 71 (1982) 345
Inequivalent methyl CH oscillators in methyl-substituted conjugated compounds as revealed by higher overtone spectra, R. Nakagaki and I. Hanazaki 72 (1982) 93
Molecular dynamics computer simulation of liquid dichloromethane. I. Equilibrium properties, M. Ferrario and M.W. Evans 72 (1982) 141
Computer simulation of dichloromethane. II. Molecular dynamics, M. Ferrario and M.W. Evans 72 (1982) 147
A new extended diffusion model for rotational motion of symmetric-top molecules in the liquid phase, J. Lascombe, M. Besnard and P. Maraval 72 (1982) 177
Ab initio study on cyanamide and isocyanamide, K. Ichikawa, Y. Hamada, Y. Sugawara, M. Tsuboi, S. Kato and K. Morokuma 72 (1982) 301
Raman scattering study of toluene vibrational relaxation in benzene–toluene liquid system, W. Reimschüssel, H. Abramczyk, H. Barańska and A. Łabudzinska 72 (1982) 313
Laser-induced ultrasonics: a dynamics holographic approach to the measurement of weak absorptions, optoelastic constants and acoustic attenuation, R.J.D. Miller, R. Casalegno, K.A. Nelson and M.D. Fayer 72 (1982) 371
Use of computer simulation to determine the triplet distribution function in dense fluids, S. Gupta, J.M. Haile and W.A. Steele 72 (1982) 425

Muonium-substituted organic free radicals in liquids. Muon–electron hyperfine coupling constants and the selectivity of formation of methyl- and fluorine-substituted cyclohexadienyl-type radicals, E. Roduner, G.A. Brinkman and P.W.F. Louwrier 73 (1982) 117
On the structure and dynamics of liquid benzene, O. Steinhauser 73 (1982) 155
Chiral discrimination in the liquid state: a hard-core model for the rôle of repulsive forces, D.P. Craig and I.R. Elsum 73 (1982) 349
Molecular interactions and reorientational motion of neat acetone in the liquid state. ^{17}O NMR chemical shifts and linewidths at variable temperature, B. Ancian, B. Tiffon and J.-E. Dubois 74 (1983) 171
Acoustic study of a critical binary mixture of nitrobenzene and *n*-hexane at low and ultrasonic frequencies, H. Tanaka, Y. Wada and H. Nakajima 75 (1983) 37
The ESR spectrum of the C_5F_5 radical, T. Chen (Dschen), F. Graf and Hs.H. Günthard 75 (1983) 165
Nickel porphyrin photophysics and photochemistry. A picosecond investigation of ligand binding and release in the excited state, D. Kim, C. Kirmaier and D. Holten 75 (1983) 305
Resonance Rayleigh light scattering of some porphyrins in solution: intensities and depolarization ratios, J. Anglister and I.Z. Steinberg 75 (1983) 443
Binary theory of dephasing in liquid solutions. II. Motion-transformed isotropic Raman spectra, A.A. Kipriyanov, A.B. Doktorov and A.K. Burshtein 76 (1983) 163
The temperature dependence of the structure of water, P.A. Egelstaff and J.H. Root 76 (1983) 405
Space- and time-resolved resonance-enhanced vibrational Raman spectroscopy from a femtosecond-lived singlet excited state of β-carotene, L.V. Haley and J.A. Koningstein 77 (1983) 1
Isothermal–isobaric molecular dynamics, D.J. Evans and G.P. Morriss 77 (1983) 63
Two-photon ionization and dissociation of liquid water by powerful laser UV radiation, D.N. Nikogosyan, A.A. Oraevsky and V.I. Rupasov 77 (1983) 131
The determination of thermal conductivity coefficients of liquids by a thermal lens technique, R.T. Bailey, F.R. Cruickshank, D. Pugh, S. Guthrie, A. McLeod, W.S. Foulds, W.R. Lee and S. Venkatesh 77 (1983) 243
Raman spectroscopic studied on the dynamics of a molecular "probe" (methyl iodide) in hydrocarbon solvents, W.F. Pacynko, J. Yarwood and D.J. Gardiner 78 (1983) 319
Comparisons between experimental argon and Lennard-Jones 12:6 shear viscosities, D. Fincham and D.M. Heyes 78 (1983) 425
Temperature dependence of J-band aggregate of the dye 1,1′-diethyl-2,2′-cyanine bromide studied by steady-state and time-resolved picosecond fluorescence spectroscopy, Z.X. Yu, P.Y. Lu and R.R. Alfano 79 (1983) 289
On the dielectric theory and computer simulation of water, O. Steinhauser 79 (1983) 465
Charge transfer in polar media. Transition-state entropy, Yu.I. Dakhnovskii and A.A. Ovchinnikov 80 (1983) 17

Solutions

Theory of optically detected magnetic resonance spectra of radical pairs, A.B. Doktorov, O.A. Anisimov, A.I. Burshtein and Yu.N. Molin 71 (1982) 1
C-13 magnetic relaxation rates and H-1 and C-13 paramagnetic shifts of Ni(II) complex of dopamine, A. Lai, M. Monduzzi, G. Saba, M. Casu and G. Crisponi 71 (1982) 271
α-hydroxyalkyl radicals by photoreduction in aprotic solvents: ESR spectra, ab initio potential function, inversion–internal rotation, dynamics and temperature dependence of coupling constants of 1-hydroxyethyl, G. Cirelli, T.-K. Ha, R. Meyer and Hs.H. Günthard 72 (1982) 15
Ab initio study on cyanamide and isocyanamide, K. Ichikawa, Y. Hamada, Y. Sugawara, M. Tsuboi, S. Kato and K. Morokuma 72 (1982) 301

A study of picosecond dehalogenation of chlorobenzene anions in liquids by positronium inhibition measurements, G. Wikander and O.E. Mogensen 72 (1982) 407
Photon-induced molecular charge separation studied by nanosecond time-resolved microwave conductivity, M.P. de Haas and J.M. Warman 73 (1982) 35
Picosecond study of pinacyanol photophysics, J.C. Mialocq 73 (1982) 107
Influence of the molecular environment in solution measurements of the second-order optical susceptibility for urea and derivatives, I. Ledoux and J. Zyss 73 (1982) 203
Positronium yields in liquids determined by lifetime and angular correlation measurements, O.E. Mogensen and F.M. Jacobsen 73 (1982) 223
Raman spectroscopy from a picosecond-lived excited state of methyl orange, L.V. Haley and J.A. Koningstein 73 (1982) 263
Picosecond kinetics of radiationless relaxation of triphenyl methane dyes. Evidence for rapid excited-state equilibrium between states of differing geometry, V. Sundström, T. Gillbro and H. Bergström 73 (1982) 439
Vibrational relaxation of hydrogen-bonded species in solution. IV. Temperature and concentration dependence of the ν_σ(OH---N) band of phenol–pyridine, U.P. Agarwal, R.S. Green and J. Yarwood 74 (1983) 35
Non-hydrodynamic contribution to the concentration dependence of the self diffusion of interacting brownian macroparticles, G.D.J. Phillies 74 (1983) 197
Chemical effects in diffusion and structure of zinc chloride in aqueous solution, A.J. Easteal, P.V. Giaquinta, N.H. March and M.P. Tosi 76 (1983) 125
Solvent effects on the potential energy surfaces of molecular iodine: a spectroscopic study, M. Geilhaupt and Th. Dorfmüller 76 (1983) 443
Inhibition of Ps formation in benzene and cyclohexane by CH_3Cl and CH_3Br. Correlation to radiation chemistry results, G. Wikander, O.E. Mogensen and N.-J. Pedersen 77 (1983) 159
Dependence of photochemical and photophysical hole burning on laser intensity, A.U. Jalmukhambetov and I.S. Osad'ko 77 (1983) 247
An NMR relaxation study of hydrogen exchange and its deuterium isotope effects in aqueous carboxylic acid solutions, D. Lankhorst, J. Schriever and J.C. Leyte 77 (1983) 319
Charge transfer to a solvent state. VII. Localization of charge during the transition state of the solute: the solute cation localization energy, T.B. Truong 77 (1983) 377
Accessibility of the lowest quintet state of organic molecules through triplet–triplet annihilation; an INDO CI study, B. Dick and B. Nickel 78 (1983) 1
Adiabatic compressibility of critical binary mixtures of nitroethane/isooctane and nitroethane/3-methylpentane, H. Tanaka and Y. Wada 78 (1983) 143
Bifurcation diagrams for two substrate oscillatory systems, J. Masełko 78 (1983) 381
Viscosity dependence of internal conversion rates of polyatomic molecules, K.-E. Süsse, D.-G. Welsch and I. Madzgalla 78 (1983) 443
On the theory of adiabatic electron-transfer reactions in polar solvents, A.B. Helman 79 (1983) 235
The theory of transitions between electronic states. Application to radiationless transitions in polar solvents, L.D. Zusman 80 (1983) 29
On the nature of the fluorescent state of methylated indole derivatives, S.R. Meech, D. Phillips and A.G. Lee 80 (1983) 317

Crystals
Absorption spectra of volatile aromatic hydrocarbon films in the vacuum ultraviolet region, S. Hino, T. Veszprémi, K. Ohno, H. Inokuchi and K. Seki 71 (1982) 135

Inelastic neutron scattering study of low frequency motions in $[Co(C_5H_5)_2^+]$ and $[Cr(C_6H_6)_2^+]$ intercalated in the $MnPS_3$ layered compound, C. Sourisseau, Y. Mathey and C. Poinsignon 71 (1982) 257
Synchrotron-radiation photoemission study of the V–VI layered compounds Bi_2Te_3, Bi_2Se_3, Sb_2Te_3 and Sb_2Te_2Se, M.R. Thuler, R.L. Benbow and Z. Hurych 71 (1982) 265
Photon echoes stimulated from long-lived ordered populations in multi-level systems. The effect of intersystem crossing and optical branching, J.B.W. Morsink, W.H. Hesselink and D.A. Wiersma 71 (1982) 289
Photochemical control of energy transfer in molecular crystals, J.S. Patel and D.M. Hanson 72 (1982) 35
X-ray photoemission and optical spectra of $NiPS_3$, $FePS_3$ and $ZnPS_3$, M. Piacentini, F.S. Khumalo, G. Leveque, C.G. Olson and D.W. Lynch 72 (1982) 61
Low-temperature vibronic spectra of 1,1′-binaphthyl, M.J. Riley, A.R. Lacey, M.G. Sceats and R.G. Gilbert 72 (1982) 83
Polymerization of TS-12 diacetylene crystals: crystal structures of monomer and polymer and spectroscopy of reaction intermediates, D. Siegel, H. Sixl, V. Enkelmann and G. Wenz 72 (1982) 201
Relativistically parameterized extended Hückel calculations. VII. Nuclear spin -spin coupling tensors and densities of states for cluster models of CdTe, HgTe and PbTe, A. Viste, M. Hotokka, L. Laaksonen and P. Pyykkö 72 (1982) 225
Phonon spectra and structure of crystalline ethylene oxide and ethylene sulphide at 77 K, R. Cataliotti and G. Paliani 72 (1982) 293
Calculations on the mechanism of ion polymerization in the formaldehyde crystal, M.V. Basilevsky, G.N. Gerasimov and S.I. Petrochenko 72 (1982) 349
Diamagnetic anisotropy of molecular complexes of 1,3,5-trinitrobenzene with anthracene and carbazole, R. Burzyński and T. Luty 72 (1982) 441
The motion of triplet excitons in β-phase crystals of 9,10-dichloroanthracene, R. Krauss, W. Schrof, H.C. Wolf and D. Schmid 73 (1982) 55
α- and β-phases of oxalic acid, $H_2C_2O_4$: vibrational spectra, normal-coordinate calculations, and intermolecular forces, J. de Villepin, A. Novak and D. Bougeard 73 (1982) 291
High-resolution absorption spectra of diphenylmethylenes, D.J. Graham and T.-S. Lin 73 (1982) 411
Semiclassical theory for atom–surface scattering: calculations on Ar + W(110), G.D. Billing 74 (1983) 143
Anharmonic processes in molecular crystals. Calculation of the anharmonic shifts, band-widths and energy processes in crystalline naphthalene, R.G. Della Valle, P.F. Fracassi, R. Righini and S. Califano 74 (1983) 179
Electrostatic energy of vacancy formation in crystals of polar molecules, R.W. Munn 74 (1983) 301
Polarization energy of a localized charge in a molecular crystal. IV. Effect of polarizability changes, I. Eisenstein, R.W. Munn and P.J. Bounds 74 (1983) 307
Theoretical model for calculations of infrared and Raman band profiles of strong hydrogen bonds in ordered media, F. Fillaux 74 (1983) 395
Calculations of infrared and Raman band profiles of strong hydrogen bonds. OH stretching bands and proton dynamics in crystalline potassium hydrogen carbonate, F. Fillaux 74 (1983) 405
Jahn–Teller splitting of the 3s → 3p transition of sodium isolated in a xenon matrix, J. Hormes and J. Schiller 74 (1983) 433
Charge-transfer transitions in crystalline anthracene and their role in photoconductivity, L. Sebastian, G. Weiser, G. Peter and H. Bässler 75 (1983) 103
A model of localization, soliton propagation, and self-trapping in an electronically excited atomic lattice, M.A. Collins and D.P. Craig 75 (1983) 191
Are new chemical species in anthracene crystals formed as a result of charge-carrier trapping at physical defects?, Z. Zboiński 75 (1983) 297

Fractionally charged ions in crystal lattices of organic ion-radical salts, L. Komorowski 76 (1983) 31
A model for the interpretation of the electronic spectra of the complex ions $M(bpy)_3^{2+}$ (M = Fe, Ru, Os) in D_3 and C_2 sites, J. Ferguson and F. Herren 76 (1983) 45
Ionization potentials and polarization energies of tetraselenafulvalene (TSF) derivatives determined from ultraviolet photoelectron spectroscopy, N. Sato, G. Saito and H. Inokuchi 76 (1983) 79
Unified theory of the electronic Stark effect in molecular crystals, R.W. Munn 76 (1983) 243
The shape of the Lorentz cavity and the internal field in anisotropic fluids, D.A. Dunmur and R.W. Munn 76 (1983) 249
Neutron scattering study of the reorientational motions in $Cr(CO)_3(\eta^6C_6H_6)$ and $Mn(CO)_3(\eta^5C_5H_5)$, G. Lucazeau, K. Chhor, C. Sourisseau and A.J. Dianoux 76 (1983) 307
A XANES study of mixed-valence transition-metal oxides and rare-earth alloys, G. Sankar, P.R. Sarode and C.N.R. Rao 76 (1983) 435
Optical activity of oriented molecules. IX. Phenomenological Mueller matrix description of thick samples and of optical elements, A. Schönhofer, H.-G. Kuball and C. Puebla 76 (1983) 453
Some problems of recombination kinetics. I, E. Kotomin and V. Kuzovkov 76 (1983) 479
Polarization energy of a localized charge in a molecular crystal. V. Effect of vacancies, I. Eisenstein and R.W. Munn 77 (1983) 47
Isothermal–isobaric molecular dynamics, D.J. Evans and G.P. Morriss 77 (1983) 63
Fermi resonance and bandshapes in deuterated palmitic acid, P. Piaggio, G. Dellepiane, R. Tubino and L. Piseri 77 (1983) 185
Delayed-fluorescence ODMR and EPR studies of triplet excitons in charge-transfer molecular crystals, G. Agostini, C. Corvaja, G. Giacometti and L. Pasimeni 77 (1983) 233
Spectroscopic studies of the photochromism of N-salicylideneaniline mixed crystals and glasses, D. Higelin and H. Sixl 77 (1983) 391
Accessibility of the lowest quintet state of organic molecules through triplet–triplet annihilation; an INDO CI study, B. Dick and B. Nickel 78 (1983) 1
Phosphorescence and E-type delayed fluorescence from azulene in phenazine host crystals, D. Klemp and B. Nickel 78 (1983) 17
Driven-echo and rotary-echo measurements of the spin coherence in triplet-state benzophenone, R. Gillies and A.M. Ponte Goncalves 78 (1983) 49
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. II. Isotopic effect, H.A. Kołodziej and S. Sorriso 78 (1983) 75
Dynamics of energy transport in ternary molecular solids. II. Time evolution of naphthalene fluorescence, P. Argyrakis and R. Kopelman 78 (1983) 251
Triplet-state optical spectra of highly concentrated isotopically mixed crystals of anthracene A-h_{10}:A-d_{10}, D. Rund and H. Port 78 (1983) 357
The effect of molecular excitation on crystal packing. 9-cyano- and 9,10-dimethylanthracene as excited guest/host and host/guest pairs, K. Norris, P. Gray, D.P. Craig, C.P. Mallett and B.R. Markey 79 (1983) 9
A quantitative analysis of the ν_s (IR) bands of H-bonds. II. Adipic acid crystals, Y. Marechal 79 (1983) 85
Polarization energy of a localized charge in a molecular crystal. VI. Effect of excitons, I. Eisenstein and R.W. Munn 79 (1983) 189
Ab initio studies on hydrogen-bonded chains. III. The linear, infinite chain of hydrogen cyanide molecules, A. Karpfen 79 (1983) 211
Spectroscopic properties of Er^{3+} ions in Li(Er, Gs)P_4O_{12} single crystals – fluorescence, Raman and infrared spectra, Z. Mazurak, J. Hanuza, K. Hermanowicz, B. Jeżowska-Trzebiatowska, D. Schultze and Ch. Waligora 79 (1983) 255
Band-state interpretation of lattice thermal conductivity and microhardness of ternary chalcopyrite semiconductors, L.K. Samanta, D.K. Ghosh and G.C. Bhar 79 (1983) 361

The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. I. Single-crystal polarized absorption spectrum, J. Baiardo, M. Vala and I. Trabjerg 79 (1983) 391
Theory of coherence effects in time-dependent delayed fluorescence. II. Application to two- and three-dimensional crystals, A. Fort, V. Ern and V.M. Kenkre 80 (1983) 205
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. III. Single-crystal Zeeman spectroscopy, J. Baiardo, M. Vala and I. Trabjerg 80 (1983) 305

Glasses and liquid crystals
Computer simulation studies of anisotropic systems. IX. The Maier–Saupe theory for nematic liquid crystals and the molecular field approximation, G.R. Luckhurst, S. Romano and P. Simpson 73 (1982) 337
Kinetics of methyl radical reaction with methanol at 20–105 K, V.L. Vyazovkin, B.V. Bol'shakov and V.A. Tolkatchev 75 (1982) 11
The ESR spectrum of the C_5F_5 radical, T. Chen (Dschen), F. Graf and Hs.H. Günthard 75 (1983) 165
Measurement of the ^{14}N nuclear quadrupole couplings in the lowest ($n\pi^*$) excited triplet state of pyrazine by ODMR, W. Fröhling, C.J. Winscom and K. Möbius 75 (1983) 389
The shape of the Lorentz cavity and the internal field in anisotropic fluids, D.A. Dunmur and R.W. Munn 76 (1983) 249
Optical activity of oriented molecules. IX. Phenomenological Mueller matrix description of thick samples and of optical elements, A. Schönhofer, H.-G. Kuball and C. Puebla 76 (1983) 453
Electron spin echo decay kinetics of an ion track in β-irradiated frozen solution of sulfuric acid. Numerical simulation by the Monte Carlo method and experiment, A.M. Raitsimring and V.V. Tregub 77 (1983) 123
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type I. Ferroelectric behaviour, H.A. Kołodziej and S. Sorriso 77 (1983) 341
The kinetics of the retarded reaction of free radicals with oxygen in a methanol glass, V.A. Bagryansky, V.M. Zaskul'nikov and V.A. Tolkatchev 78 (1983) 41
Dispersive singlet motion in an organic glass, R. Jankowiak and H. Bässler 79 (1983) 57
Temperature dependence of J-band aggregate of the dye 1,1′-diethyl-2,2′-cyanine bromide studied by steady-state and time-resolved picosecond fluorescence spectroscopy, Z.X. Yu, P.Y. Lu and R.R. Alfano 79 (1983) 289
Singlet exciton migration in a random organic two-component system containing physical and chemical traps, G. Peter, B. Ries and H. Bässler 80 (1983) 289

Metals
Magnetic resonance experiments on the radical cation salt $(fluoranthenyl)_2^+PF_6^-$. Correlation of proton-NMR, fluorine-NMR and ESR, W. Höptner, M. Mehring, J.U. von Schütz, H.C. Wolf, B.S. Morra, V. Enkelmann and G. Wegner 73 (1982) 253
Van der Waals forces and molecular diffraction from metal surfaces, with application to Ag(111), N.R. Hill, M. Haller and V. Celli 73 (1982) 363
X-ray structure and optical properties of silver films prepared by condensation or preformed Ag-clusters, W. Vogel, B. Tesche and W. Schulze 74 (1983) 137

Semiconductors
Inelastic neutron scattering study of low frequency motions in $[Co(C_5H_5)_2^+]$ and $[Cr(C_6H_6)_2^+]$ intercalated in the $MnPS_3$ layered compound, C. Sourisseau, Y. Mathey and C. Poinsignon 71 (1982) 257
Synchrotron-radiation photoemission study of the V–VI layered compounds Bi_2Te_3, Bi_2Se_3, Sb_2Te_3 and Sb_2Te_2Se, M.R. Thuler, R.L. Benbow and Z. Hurych 71 (1982) 265

X-ray photoemission and optical spectra of $NiPS_3$, $FePS_3$ and $ZnPS_3$, M. Piacentini, F.S. Khumalo, G. Leveque, C.G. Olson and D.W. Lynch 72 (1982) 61
Magnetic resonance experiments on the radical cation salt $(fluoranthenyl)_2^+PF_6^-$. Correlation of proton-NMR, fluorine-NMR and ESR, W. Höptner, M. Mehring, J.U. von Schütz, H.C. Wolf, B.S. Morra, V. Enkelmann and G. Wegner 73 (1982) 253
Comparative reinvestigation of the interaction of phonons with Wannier and Frenkel excitons in crystalline solids, J. Singh 75 (1983) 371
On a site-selective EXAFS experiment using optical emission, J. Goulon, P. Tola, M. Lemonnier and J. Dexpert-Ghys 78 (1983) 347
Band-state interpretation of lattice thermal conductivity and microhardness of ternary chalcopyrite semiconductors, L.K. Samanta, D.K. Ghosh and G.C. Bhar 79 (1983) 361

Surfaces
Theoretical studies of ion neutralization: two-dimensional tight binding models, H.K. McDowell 72 (1982) 451
Satellites in the X-ray photoelectron spectra of transition-metal and rare-earth compounds, D.D. Sarma, P. Vishnu Kamath and C.N.R. Rao 73 (1982) 71
Van der Waals forces and molecular diffraction from metal surfaces, with application to Ag(111), N.R. Hill, M. Haller and V. Celli 73 (1982) 363
Reactions induced by ion bombardment of solid cyclohexane at 77 K, O. Puglisi, G. Marletta, S. Pignataro and G. Foti 75 (1983) 417
An extended Hückel study of hydrogen and oxygen chemisorption on Ru(001) surface, B.C. Khanra and S.K. Saha 76 (1983) 255
Comparison of photon-stimulated dissociation of gas-phase, solid and chemisorbed water, D.E. Ramaker 80 (1983) 183

Dielectrics
Polarization energy of a localized charge in a molecular crystal. IV. Effect of polarizability changes, I. Eistenstein, R.W. Munn and P.J. Bounds 74 (1983) 307
Are new chemical species in anthracene crystals formed as a result of charge-carrier trapping at physical defects?, Z. Zboiński 75 (1983) 297
The shape of the Lorentz cavity and the internal field in anisotropic fluids, D.A. Dunmur and R.W. Munn 76 (1983) 249
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. I. Ferroelectric behavior, H.A. Kołodziej and S. Sorriso 77 (1983) 341
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. II. Isotopic effect, H.A. Kołodziej and S. Sorriso 78 (1983) 75
Polarization energy of a localized charge in a molecular crystal. VI. Effect of excitons, I. Eisenstein and R.W. Munn 79 (1983) 189
Secondary amines: a low-temperature dielectric relaxation study, J. Gilchrist and H. Godfrin 79 (1983) 307
Dipole–phonon coupling and dielectric relaxation, R. Nigmatullin and L.A. Dissado 79 (1983) 455
On the dielectric theory and computer simulation of water, O. Steinhauser 79 (1983) 465
Charge transfer in polar media. Transition-state entropy, Yu.I. Dakhnovskii and A.A. Ovchinnikov 80 (1983) 17
Primary amines: a low-temperature dielectric relaxation study, J. Gilchrist 80 (1983) 63

Plasmas
Spectroscopic analysis of the vibrational distributions in dissociative CO–He RF discharges, S. de Benedictis, R. d'Agostino and F. Cramarossa 71 (1982) 247

Turbulence in fluids and plasmas, D. ter Haar 71 (1982) 345
Collision dominated relaxation of electrons in a weakly ionized nitrogen plasma after abrupt change of the electric field, M. Capitelli, C. Gorse, J. Wilhelm and R. Winkler 79 (1983) 1
Can the H_5 molecule be observed?, K. Kaufmann, M. Jungen and V. Staemmler 79 (1983) 111

Microscopic systems

Atoms

X-ray scattering factors, Compton profiles, and shell corrections from numerical atomic wavefunctions, J. Oddershede and J.R. Sabin 71 (1982) 161
Electronic properties by Green's function calculations. Renormalized optical potential results: Ne, Ar, HF, H_2O, NH_3, I. Cacelli, R. Moccia and V. Carravetta 71 (1982) 199
Dynamics polarizability of many-electron systems with a time-dependent density-functional theory, S.K. Ghosh and B.M. Deb 71 (1982) 295
Time-resolved spectroscopy: wavepacket formalism in the coherent-state representation, A.A. Villaeys and K.F. Freed 72 (1982) 1
Atoms-in-molecules calculations on dynamic fragments of polyatomic systems: HeH, HeH^+ and HeH^- for a DIM model of Penning ionization of H_2 by He^*, I. Paidarová, J. Vojtík and R. Polák 72 (1982) 119
A spin-adapted linear response theory in a coupled-cluster framework for direct calculation of spin-allowed and spin-forbidden transition energies, S. Ghosh, D. Mukherjee and S.N. Bhattacharyya 72 (1982) 161
Collision-induced absorption in a He–Ar mixture, A. Raczyński 72 (1982) 321
Glory undulations in the total cross section for Ar–Ar,Kr,Xe and Kr–Ar,Kr, H.C.W. Beijerinck, P.M.A. van der Kam and N.F. Verster 72 (1982) 391
Microphone detection of pulsed atomic and molecular beams, J.G. Choi and G.J. Diebold 73 (1982) 19
Semiclassical theory for atom–surface scattering: calculations on Ar + W(110), G.D. Billing 74 (1983) 143
Jahn–Teller splitting of the 3s → 3p transition of sodium isolated in a xenon matrix, J. Hormes and J. Schiller 74 (1983) 433
Fluorescence from the a ^5P and a ^3P states of matrix-isolated Fe atoms, M.T. McKenzie Jr. and F.R. Nixon 75 (1983) 115
Local normal modes and vibrational adiabatic potentials, N. Agmon 76 (1983) 203
Dynamics of a prototype alkali–hydrogen-halide exchange reaction on an ab initio potential-energy surface, I. NoorBatcha and N. Sathyamurthy 77 (1983) 67
Generalized Landau–Zener formula for non-adiabatic transitions between degenerate states, V.V. Likhansky and G.A. Solodovnikov 77 (1983) 409
Eigenvalues of the Boltzmann collision operator for binary gases: relaxation of anisotropic distributions, B. Shizgal and R. Blackmore 77 (1983) 417
Finite-field many-body perturbation theory. VI. Multipole polarizabilities of beryllium. A comparative study, G.H.F. Diercksen and A.J. Sadlej 77 (1983) 429
Surface hopping trajectory calculations for electronic rotational and vibrational inelastic collisions for the Na–N_2 system, P. Archirel and P. Habitz 78 (1983) 213
Interaction potentials for Li^+–rare-gas systems, L.A. Viehland 78 (1983) 279
Breathing-sphere quantum calculations of integral and differential cross sections for vibrational excitation in ion (atom)–diatom collisions, G. Drolshagen and J.P. Toennies 79 (1983) 159
Search for the laser-induced crossed beam reaction of excited $I_2(B\,^3\Pi)$ with Hg, M.M. Oprysko, F.J. Aoiz, R.B. Bernstein and M.A. McMahan 79 (1983) 341
Kinetics and detection of $F(^2P)$ atoms in a discharge flow system, M.A.A. Clyne and A. Hodgson 79 (1983) 351

Effective core potential calculations using frozen orbitals. Applications to transition metals, L.G.M. Pettersson, U. Wahlgren and O. Gropen 80 (1983) 7
Vibrational effects with excitation transfer in metastable rare-gas–halide collisions, M.S. de Vries and R.M. Martin 80 (1983) 157
Theoretical study of shake-up in the core photoelectron spectra of the alkali atoms, G. de Alti, P. Decleva and A.Lisini 80 (1983) 229

Molecules

Conformational interconversions in supersonic jets: matrix IR spectroscopy and model calculations, P. Felder and Hs.H. Günthard 71 (1982) 9
Are atoms intrinsic to molecular electronic wavefunctions? I. The FORS model, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 41
Are atoms intrinsic to molecular electronic wavefunctions? II. Analysis of FORS orbitals, K. Ruedenberg, M.W. Schmidt and M.M. Gilbert 71 (1982) 51
Are atoms intrinsic to molecular electronic wavefunctions? III. Analysis of FORS configurations, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 65
Ab initio calculation of the zero-field splitting of the $X\,^3\Sigma_g^-$ and $B\,^3\Pi_{g,i}$ states of the S_2 molecule, B.A. Hess, R.J. Buenker, C.M. Marian and S.D. Peyerimhoff 71 (1982) 79
Near-degeneracy effects and efficiency of MBPT calculations of molecular properties. Polarizability curve of H_2, G.H.F. Diercksen, M. Jaszuński and A.J. Sadlej 71 (1982) 105
Exchange reactions of hydrogen halides with hydrogenic atoms, D.C. Clary 71 (1982) 117
The application of exterior complex scaling in calculations on resonance in nuclear motion in molecular systems, J. Turner and C.W. McCurdy 71 (1982) 127
Absorption spectra of volatile aromatic hydrocarbon films in the vacuum ultraviolet region, S. Hino, T. Veszprémi, K. Ohno, H. Inokuchi and K. Seki 71 (1982) 135
Evaluation of an upper bound of the maximal Lyapunov characteristic number by Monte Carlo integration in the chaotic regions of phase space, S.C. Farantos 71 (1982) 157
The selection of coordinate systems for describing large-amplitude nuclear motion in triatomic molecules, R. Wallace 71 (1982) 173
Electronic properties by Green's function calculations. Renormalized optical potential results: Ne, Ar, HF, H_2O, NH_3, I. Cacelli, R. Moccia and V. Carravetta 71 (1982) 199
Fermi-coupled spherically adapted effective states in the collisionless multiphoton excitation of SF_6, C. di Lauro and F. Lattanzi 71 (1982) 233
Infrared multiple photon excitation of sulfur hexafluoride in a molecular beam, D. Bassi, A. Boschetti, G. Scoles, M. Scotoni and M. Zen 71 (1982) 239
Photon echoes stimulated from long-lived ordered populations in multi-level systems. The effect of intersystem crossing and optical branching, J.B.W. Morsink, W.H. Hesselink and D.A. Wiersma 71 (1982) 289
Dynamic polarizability of many-electron systems within a time-dependent density-functional theory, S.K. Ghosh and B.M. Deb 71 (1982) 295
A semiclassical model for the vibrational excitation of spherical-top molecules in collisions with ions, T. Ellenbroek and J.P. Toennies 71 (1982) 309
Analysis of the steric dependence of the CH_3I + Rb reaction using a Legendre expansion technique, S. Stolte, K.K. Chakravorty, R.B. Bernstein and D.H. Parker 71 (1982) 353
On the use of "effective harmonic potentials" and "effective normal coordinates" in computing the vibrational energy levels of polyatomic molecules, G. Amat 71 (1982) 363
The vibrational energy manifold of the lowest lying bending mode of tricarbon oxide sulfide, O=C=C=C=S, as determined by relative intensity measurements, M. Winnewisser and E.W. Peau 71 (1982) 377

Avoided-crossing molecular-beam spectroscopy of CH_3SiF_3, W.L. Meerts and I. Ozier 71 (1982) 401
Superfine and hyperfine structures in the ν_3 band of $^{32}SF_6$, J. Bordé and Ch.J. Bordé 71 (1982) 417
State-to-state total cross sections for ion-pair formation, U.C. Klomp and J. Los 71 (1982) 443
Time-resolved spectroscopy: wavepacket formalism in the coherent-state representation, A.A. Villaeys and K.F. Freed 72 (1982) 1
Multiphoton dissociation of some volatile uranyl complexes. I. The phenomena of reversible and permanent dissociation, J.E. Eberhardt, I.E. Hoare, D.A. Johnson, R.B. Knott, A.W. Pryor and A.B. Waugh 72 (1982) 41
Multiphoton dissociation of some volatile uranyl complexes. II. Frequency and isotopic effects, J.E. Eberhardt, R.B. Knott and A.W. Pryor 72 (1982) 51
Highly resolved optical spectra of *o*-durylene, W.P. Cofino, G.Ph. Hoornweg, C. Gooijer, C. MacLean and N.H. Velthorst 72 (1982) 73
Inequivalent methyl CH oscillators in methyl-substituted conjugated compounds as revealed by higher overtone spectra, R. Nakagaki and I. Hanazaki 72 (1982) 93
Potential energy curves and transition moments for the low-lying electronic states of the Si_2 molecule, S.D. Peyerimhof and R.J. Buenker 72 (1982) 111
Atoms-in-molecules calculations on diatomic fragments of polyatomic systems: HeH, HeH^+ and HeH^- for a DIM model of Penning ionization of H_2 by He^*, I. Paidarová, J. Vojtík and R. Polák 72 (1982) 119
Unified theoretical treatment of analytic first and second energy derivatives in open-shell Hartree–Fock theory, Y. Osamura, Y. Yamaguchi, P. Saxe, M.A. Vincent, J.F. Gaw and H.F. Schaefer III 72 (1982) 131
A spin-adapted linear response theory in a coupled-cluster framework for direct calculation of spin-allowed and spin-forbidden transition energies, S. Ghosh, D. Mukherjee and S.N. Bhattacharyya 72 (1982) 161
A new extended diffusion model for rotational motion of symmetric-top molecules in the liquid phase, J. Lascombe, M. Besnard and P. Maraval 72 (1982) 177
Studies of magnetic field effects on the intensity and the lifetime of sulfur dioxide luminescence in the gas phase, V.I. Makarov, N.L. Lavrik and N.M. Bazhin 72 (1982) 213
Photoelectron spectra and their relativistic interpretation for gaseous bismuth trihalides, R.G. Egdell, M. Hotokka, L. Laaksonen, P. Pyykkö and J.G. Snijders 72 (1982) 237
Two-photon excitations of bond modes, M.L. Sage and J. Jortner 72 (1982) 249
Polarization of $CN(B\,^2\Sigma^+ - X\,^2\Sigma^+)$ emission produced in the electron-impact dissociation of HCN and DCN, T. Nagata, T. Kondow and K. Kuchitsu 72 (1982) 281
The structure of F_2O_2: theoretical predictions and comparisons with F_2 and F_2O, R. Ahlrichs and P.R. Taylor 72 (1982) 287
Ab initio study on cyanamide and isocyanamide, K. Ichikawa, Y. Hamada, Y. Sugawara, M. Tsuboi, S. Kato and K. Morokuma 72 (1982) 301
Raman scattering study of toluene vibrational relaxation in benzene–toluene liquid system, W. Reimschüssel, H. Abramczyk, H. Barańska and A. Łabudzinska 72 (1982) 313
Interpretation of resonance CARS and Shpolskii spectra with calculated molecular geometries, vibrational frequencies and relative intensities: chrysene in its lowest excited singlet and triplet state, Ch. Jung, A. Lau, H.-J. Weigmann, W. Werncke and M. Pfeiffer 72 (1982) 327
Random coupling models. IV. Numerical investigation of the dependence on the random coupling distribution and on the initial phases, B. Carmeli, R. Tulman, A. Nitzan and M.H. Kalos 72 (1982) 363
Electronic–vibrational excitations of a hydrogen-bonded molecule in supersonic expansions: 1,4-dihydroxyanthraquinone and its deuterated derivatives, G. Smulevich, A. Amirav, U. Even and J. Jortner 73 (1982) 1

Microphone detection of pulsed atomic and molecular beams, J.G. Choi and G.J. Diebold 73 (1982) 19
Temperature dependence of the reactions of CH radicals with unsaturated hydrocarbons, M.R. Berman, J.W. Fleming, A.B. Harvey and M.C. Lin 73 (1982) 27
Theoretical studies of the electronic spectrum of thioformaldehyde, P.G. Burton, S.D. Peyerimhoff and R.J. Buenker 73 (1982) 83
Electron impact dissociation of molecular hydrogen and deuterium: isotope effect on the emission cross section of H^* and D^* ($n = 3, 4, 5$), M. Higo, S. Kamata and T. Ogawa 73 (1982) 99
Picosecond study of pinacyanol photophysics, J.C. Mialocq 73 (1982) 107
Ab initio calculations of radiative transition probabilities in the $X\,^1\Sigma^+$ state of SiO and the $X\,^2\Sigma^+$ and $A\,^2\Pi$ states of SiO^+, H.-J. Werner, P. Rosmus and M. Grimm 73 (1982) 169
An ab initio study of relationships between bond lengths and the harmonic and anharmonic cross-coupling constants involving the double bonds in hetero-atom substituted conjugated dienes, C.W. Bock, M. Trachtman and P. George 73 (1982) 179
Influence of the molecular environment in solution measurements of the second-order optical susceptibility for urea and derivatives, I. Ledoux and J. Zyss 73 (1982) 203
Concurrence of the $n\nu_3$ and $(n-1)\nu_3 + \nu_2 + \nu_6$ vibrational ladders in the collisionless multiphoton excitation of $^{32}SF_6$, C. di Lauro, F. Lattanzi and G. Sanna 73 (1982) 215
The Franck–Condon principle for radiationless transitions in molecules and a selection rule for Morse oscillators, E.S. Medvedev 73 (1982) 243
Raman spectroscopy from a picosecond-lived excited state of methyl orange, L.V. Haley and J.A. Koningstein 73 (1982) 263
Vibrational deactivation of CO($v = 1$) by p-H_2 and o-H_2, L.L. Poulsen and G.D. Billing 73 (1982) 313
Photodissociation of molecular beams of SO_2 at 193 nm, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 73 (1982) 377
Dissociation cross sections of silane and disilane by electron impact, J. Perrin, J.P.M. Schmitt, G. de Rosny, B. Drevillon, J. Huc and A. Lloret 73 (1982) 383
Influence of the oxy, aza and thio groups on the electron affinities of carbonyl compounds studied by means of ETS, A. Modelli, G. Distefano and D. Jones 73 (1982) 395
Photochemical decay of butynal ($H_3CC{\equiv}C-CHO$) in the gas phase following $S_1(n\pi^*) \leftarrow S_0$ excitation, H.U. Zürcher, U. Brühlmann and J.R. Huber 73 (1982) 403
The dual phosphorescence of benzophenazine in ethanol, G.W. Suter and U.P. Wild 73 (1982) 421
Picosecond kinetics of radiationless relaxations of triphenyl methane dyes. Evidence for rapid excited-state equilibrium between states of differing geometry, V. Sundström, T. Gillbro and H. Bergström 73 (1982) 439
On the relativistic theory of NMR chemical shifts, P. Pyykkö 74 (1982) 1
Vibrational–translational/rotational and vibrational–vibrational processes in methane/inert-gas mixtures: optoacoustic phase measurements, E. Avramides and T.F. Hunter 74 (1983) 25
The polarization dependence of two-photon absorption rates for randomly oriented molecules, M.A.C. Nascimento 74 (1983) 51
Molecular translational–rovibronic hamiltonian. I. Non-linear molecules, R. Islampour and M. Kasha 74 (1983) 67
Spectra and emission lifetimes of $H_2CS(\tilde{A}\,^1A_2)$, M. Kawasaki, K. Kasatani, Y. Ogawa and H. Sato 74 (1983) 83
Energy-transfer reactions between He($2\,^3S$) and Ne($^3P_{0,2}$) metastable atoms and PN radicals, H. Obase, M. Tsuji and Y. Nishimura 74 (1983) 89
Quantum-mechanical rearrangement processes: off-shell vibrorotational sudden approximation to the dynamics, E. Ficocelli Varracchio 74 (1983) 153

Angle-resolved photoelectron measurements on the 2p orbitals of Si in SiF_4 and $Si(CH_3)_4$ in the gas phase, P.R. Keller, J.W. Taylor, F.A. Grimm, P. Senn, T.A. Carlson and M.O. Krause 74 (1983) 247
Absolute dipole oscillator strengths for molecular and dissociative photoionization of hydrogen fluoride, F. Carnovale and C.E. Brion 74 (1983) 253
Photofragmentation of H_2S in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 74 (1983) 261
Large-amplitude vibration in triatoms. II. Introduction of potential refinement within a LAV model applied to the sulfur dioxide molecule, R. Wallace 74 (1983) 339
Quantum vibrational transition probabilities from real classical trajectories: asymmetric diatom–diatom collisions, R.T. Skodje, W.R. Gentry and C.F. Giese 74 (1983) 347
An efficient solution of weak-collision master equations in thermal unimolecular reaction rate theory, H.W. Schranz and S. Nordholm 74 (1983) 365
Theoretical solvent effects on molecular structure and spectroscopic properties through the virtual-charge model. Application to the inverted solvatochromy of benzophenone $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ absorption bands, A. Botrel, F. Corre and A. le Beuze 74 (1983) 383
Theoretical model for calculations of infrared and Raman band profiles of strong hydrogen bonds in ordered media, F. Fillaux 74 (1983) 395
Calculations in infrared and Raman band profiles of strong hydrogen bonds. OH stretching bands and proton dynamics in crystalline potassium hydrogen carbonate, F. Fillaux 74 (1983) 405
The unimolecular dissociation of electronic state-selected methyl iodide cations, I. Powis 74 (1983) 421
The dipole moment of ^{7}LiH and ^{7}LiD in the excited $A\,^1\Sigma^+$ state: a test of the Born–Oppenheimer approximation, M. Brieger, A. Renn, A. Sodeik and A. Hese 75 (1983) 1
Classical aspects of the laser excitation of a Morse oscillator, S.K. Gray 75 (1983) 67
Semi-empirical correction to the mixing coefficients for the diatomics-in-molecules method, P.J. Kuntz and C.C. Chang 75 (1983) 79
Electronic structure of potassium clusters (K_9, K_{15}, K_{27}) by the SCF Xα(LSD) SW method, A. Pellegatti, B.N. McMaster and D.R. Salahub 75 (1983) 83
Convergence of an improved CIPSI algorithm, S. Evangelisti, J.-P. Daudey and J.-P. Malrieu 75 (1983) 91
Two-frequency CO_2 laser multiple-photon dissociation and dynamics of excited state absorption in CDF_3, I.P. Herman 75 (1983) 121
Molecular translational–rovibronic hamiltonian. II. Linear molecules, R. Islampour and M. Kasha 75 (1983) 157
Trajectory surface-hopping study of the $K + O_2$ collision: energy transfer in neutral and ionic products, G. Parlant, M. Schröder and S. Goursaud 75 (1983) 175
The semiclassical determination of potential surfaces from observed spectra. I, S.M. Colwell and I.C. Percival 75 (1983) 215
The semiclassical determination of potential surfaces from observed spectra. II, S.M. Colwell and I.C. Percival 75 (1983) 225
Vibrationally excited molecules and mechanisms of chemical and physical processes in non-equilibrium plasmas, P.A. Sergeev and D.I. Slovetsky 75 (1983) 231
The electronic structure of chalcogen hexahalogenides, G.L. Gutsev and A.P. Klyagina 75 (1983) 243
High-resolution HeI and HeII photoelectron spectra of the zinc and cadmium dihalide valence bands, D.J. Bristow, G.M. Bancroft and J.S. Tse 75 (1983) 263
High-resolution HeI and HeII photoelectron spectra of the Zn 3d and Cd 4d orbitals in the zinc and cadmium dihalides: ligand field splittings and intensity variations, G.M. Bancroft, D.J. Bristow and J.S. Tse 75 (1983) 277
Nickel porphyrin photophysics and photochemistry. A picosecond investigation of ligand binding and release in the excited state, D. Kim, C. Kirmaier and D. Holten 75 (1983) 305

Experimental and theoretical study of the vibrational relaxation of CO($v = 1$) and N_2($v = 1$): V–T relaxation by the isotopes of helium, M.M. Maricq, E.A. Gregory, C.T. Wickham-Jones, D.J. Cartwright and C.J.S.M. Simpson 75 (1983) 347
Measurement of the ^{14}N nuclear quadrupole couplings in the lowest ($n\pi^*$) excited triplet state of pyrazine by ODMR, W. Fröhling, C.J. Winscom and K. Möbius 75 (1983) 389
Molecular structure and photoelectron spectra of H_2S, H_2Se, and H_2Te. Effective core potential calculations on ground and valence ionic states, J. Müller, L.J. Sæthre and O. Gropen 75 (1983) 395
Cluster expansion of the wavefunction. Valence and Rydberg excitations, ionizations, and inner-valence ionizations of CO_2 and N_2O studied by the SAC and SAC CI theories, H. Nakatsuji 75 (1983) 425
Resonance Rayleigh light scattering of some porphyrins in solution: intensities and depolarization ratios, J. Anglister and I.Z. Steinberg 75 (1983) 443
Chaotic motions in vibrating molecules: the generalized Hénon–Heiles model, R. Ramaswamy 76 (1983) 15
On the statistics of an ensemble of oscillators under excitation. IV. Evaluation of the time for kinetic excitation into the quasicontinuum based on Kramers' theory, V.N. Sazonov and I.E. Khromov 76 (1983) 25
Molecular orbital electron momentum distributions and separation energies of CH_3CN, A. Minchinton, C.E. Brion, J.P.D. Cook and E. Weigold 76 (1983) 89
Fluorescence quenching of tertiary amines by halocarbons, P.C. Alford, C.G. Cureton, R.A. Lampert and D. Phillips 76 (1983) 103
Density functional estimates of charge transfer and chemical potentials in hydrogen halides and mixed halides, J.A. Alonso and N.H. March 76 (1983) 121
Binary theory of dephasing in liquid solutions. I. The non-markovian theory of encounters, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 149
Binary theory of dephasing in liquid solutions. II. Motion-transformed isotropic Raman spectra, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 163
The radiative lifetime of the $A\,^1\Pi$ state of CH^+ calculated from long CAS SCF expansions, M. Larsson and P.E.M. Siegbahn 76 (1983) 175
MS Xα and LCAO Xα calculations of ionization potentials. A comparison with Koopmans' theorem and accurate calculations, G. de Alti, P. Decleva and A. Lisini 76 (1983) 185
Local normal modes and vibrational adiabatic potentials, N. Agmon 76 (1983) 203
Photodissociation kinematics. II. Laboratory angular distribution of a hydride model system and the kinematic isotope effect, K.-M. Chen and C.-C. Pei 76 (1983) 219
Rate constants for vibrational energy transfer between CO ($v = 1$) and CH_4 and substituted methane molecules in the temperature range 300 to 80 K, D.C. Allen and C.J.S.M. Simpson 76 (1983) 231
Diatomic-in-molecules potential energy surfaces of $(HeH_2)^+$: an extended basis set calculation, F. Schneider, L. Zülicke, R. Polák and J. Vojtík 76 (1983) 259
Cluster expansion of the wavefunction. Outer- and inner-valence ionization spectra of CS_2 and COS, H. Nakatsuji 76 (1983) 283
Spectroscopic investigation of the electronic structure of the chlorine molecule in the VUV, Th. Moeller, B. Jordan, P. Gürtler, G. Zimmerer, D. Haaks, J. de Calve and M.-C. Castex 76 (1983) 295
Semiclassical calculation of energy transfer in polyatomic molecules. VIII. Theory for atom + non-linear triatom, G.D. Billing 76 (1983) 315
New type of rotational basis function for quantum-mechanical molecular collision calculations, D.C. Clary 76 (1983) 331
Comment on collisionless vibrational relaxation, W. Fuss 76 (1983) 343
The description of molecular large-amplitude motions in terms of curvilinear coordinates associated with the reaction path, A. Nauts and X. Chapuisat 76 (1983) 349

Study of the dependence of spin–orbit matrix elements on AO basis set composition for inner and valence shells: results for the multiplet splitting of $X\,^3\Sigma^-$ and $C\,^3\Pi$ of SO and $X\,^2\Pi$ in SO^+, R. Klotz, C.M. Marian, S.D. Peyerimhoff, B.A. Hess and R.J. Buenker 76 (1983) 367
Large-amplitude vibration in triatoms. III. Application to linear molecules: vibrational states of HCN, R. Wallace 76 (1983) 421
The N1s shake-up spectrum of para-aminobenzonitrile. A theoretical and experimental ESCA study, P.-Å. Malmquist, S. Svensson and H. Ågren 76 (1983) 429
Solvent effects on the potential energy surfaces of molecular iodine: a spectroscopic study, M. Geilhaupt and Th. Dorfmüller 76 (1983) 443
The dissociation energies of gaseous SmLi, EuLi, TmLi and YbLi, A. Neubert and K.F. Zmbov 76 (1983) 469
Space- and time-resolved resonance-enhanced vibrational Raman spectroscopy from a femtosecond-lived singlet excited state of β-carotene, L.V. Haley and J.A. Koningstein 77 (1983) 1
Infrared-induced conformational isomerization of ethylene glycol in a low-temperature argon matrix, H. Takeuchi and M. Tasumi 77 (1983) 21
Vibronic and multimode effects on the Raman excitation profile of a totally symmetric fundamental in the Soret band of cytochrome c, W. Siebrand and M.Z. Zgierski 77 (1983) 35
Dynamics of a prototype alkali hydrogen-halide exchange reaction on an ab initio potential-energy surface, I. NoorBatcha and N. Sathyamurthy 77 (1983) 67
Perturbation theory of the electron correlation effects for atomic and molecular properties. VI. Complete active space (CAS) SCF and MBPT calculations of electric properties of the FH molecule, G.H.F. Diercksen, V. Kellö, B.O. Roos and A.J. Sadlej 77 (1983) 93
Two-photon ionization and dissociation of liquid water by powerful laser UV radiation, D.N. Nikogosyan, A.A. Oraevsky and V.I. Rupasov 77 (1983) 131
Intensities in inelastic neutron scattering spectra: a test of recent theory, J. Howard, B.C. Boland and J. Tomkinson 77 (1983) 145
The nature of the stabilizing effect of thio groups on the Π anion states of benzene studied by means of electron transmission spectroscopy, A. Modelli, D. Jones, F.P. Colonna and G. Distefano 77 (1983) 153
Raman analysis of SF_6 molecular beams excited by a cw CO_2 laser, G. Luijks, J. Timmerman, S. Stolte and J. Reuss 77 (1983) 169
Electronic spectra of jet-cooled azulene, M. Fujii, T. Ebata, N. Mikami and M. Ito 77 (1983) 191
Relaxation and spectroscopy of CaCl in seeded supersonic beams, U. Buck, J. Kesper, H.H. Kuge and D. Otten 77 (1983) 201
The role of tautomeric and rotameric species in the photophysics of 2-(2′-hydroxyphenyl)-benzoxazole, G.J. Woolfe, M. Melzig, S. Schneider and F. Dörr 77 (1983) 213
Dynamics of formation of $CN(B\,^2\Sigma^+)$ fragment from HCN and DCN in an argon afterglow, Y. Ozaki, T. Kondow and K. Kuchitsu 77 (1983) 223
Oscillator strengths and lifetimes of the C_2 $A\,^1\Pi_u$–$X\,^1\Sigma_g^+$ Phillips system, E.F. van Dishoeck 77 (1983) 277
Monte Carlo calculations on unimolecular reactions, energy transfer, and IR-multiphoton decomposition, J.R. Barker 77 (1983) 301
Ultrafast non-radiative decay via conical intersections of molecular potential-energy surfaces: $C_2H_4^+$, H. Köppel 77 (1983) 359
Spectroscopic studies of the photochromism of N-salicylideneaniline mixed crystals and glasses, D. Higelin and H. Sixl 77 (1983) 391
Generalized Landau Zener formula for non-adiabatic transitions between degenerate states, V.V. Likhansky and G.A. Solodovnikov 77 (1983) 409
Eigenvalues of the Boltzmann collision operator for binary gases: relaxation of anisotropic distributions, B. Shizgal and R. Blackmore 77 (1983) 417

Phosphorescence and E-type delayed fluorescence from azulene in phenazine host crystals, D. Klemp and B. Nickel 78 (1983) 17
He–HF vibrational inelasticity at low and intermediate energies from quantum collision theory, F.A. Gianturco, U.T. Lamanna and G. Petrella 78 (1983) 81
Theoretical three-dimensional potential-energy surface for the reaction of Be with HF, S. Chapman, M. Dupuis and S. Green 78 (1983) 93
Atoms-in-molecules study of ground- and excited-state potential-energy curves for Li_2, R. Polák and J. Vojtík 78 (1983) 107
Complete valence-shell ionization spectra of N_2 and CO: application of the extended two-particle–hole Tamm–Dancoff approximation (2ph-TDA), J. Schirmer and O. Walter 78 (1983) 201
Surface hopping trajectory calculations for electronic rotational and vibrational inelastic collisions for the Na–N_2 system, P. Archirel and P. Habitz 78 (1983) 213
Semiclassical theory of predissociation induced by rotational (Coriolis) coupling, H. Nakamura 78 (1983) 235
Non-Condon scheme of radiationless transitions for the Morse oscillator model, A.L. Sobolewski 78 (1983) 265
Infrared laser photoisomerization of 2-fluoroethanol in argon, W.F. Hoffman III and J.S. Shirk 78 (1983) 331
On a site-selective EXAFS experiment using optical emission, J. Goulon, P. Tola, M. Lemonnier and J. Dexpert-Ghys 78 (1983) 347
Triplet-state optical spectra of highly concentrated isotopically mixed crystals of anthracene A-h_{10}:A-d_{10}, D. Rund and H. Port 78 (1983) 357
The $B\,^2\Sigma^+$–$X\,^2\Sigma^+$ system of SrF: precise spectroscopic constants from a combined fit of microwave and sub-Doppler optical spectra, W.E. Ernst and J.O. Schröder 78 (1983) 363
State-selected molecular-beam reaction dynamics of K with HF ($v = 1$, $j = 5,6$ and 7), M. Hoffmeister, L. Potthast and H.J. Loesch 78 (1983) 369
Hartree–Fock–Slater LCAO calculation of the Mössbauer parameters of some antimony compounds, W. Ravenek, J.W.M. Jacobs and A. van der Avoird 78 (1983) 391
Valence-shell photoabsorption by CO_2 and its connections with electron–CO_2 scattering, P.M. Dittman, D. Dill and J.L. Dehmer 78 (1983) 405
Viscosity dependence of internal conversion rates of polyatomic molecules, K.-E. Süsse, D.-G. Welsch and I. Madzgalla 78 (1983) 443
Collision dominated relaxation of electrons in a weakly ionized nitrogen plasma after abrupt change of the electric field, M. Capitelli, C. Gorse, J. Wilhelm and R. Winkler 79 (1983) 1
A quantitative analysis of the ν_s(IR) bands of H-bonds. I. Theory, Y. Marechal 79 (1983) 69
Measurements of depolarization ratios of gaseous linear chain molecules: a test of the principle of the additivity of bond polarizabilities, J.E.M. Haverkort, F. Baas and J.J.M. Beenakker 79 (1983) 105
A comparison of quantal and semiclassical perturbed-rotational-state methods in H^+–CO collisions, K. Sakimoto 79 (1983) 137
Theoretical investigation of rotational rainbows in K + N_2 and K + CO collisions, D. Häusler and R. Schinke 79 (1983) 147
Breathing-sphere quantum calculations of integral and differential cross sections for vibrational excitation in ion (atom)–diatom collisions, G. Drolshagen and J.P. Toennies 79 (1983) 159
Semiclassical calculation of energy transfer in polyatomic molecules. X. Energy transfer in Ar + SF_6 at 1 eV, G.D. Billing 79 (1983) 179
Prediction and interpretation of collinear reactive scattering resonances by the diagonal corrected vibrational adiabatic hyperspherical model, J. Römelt 79 (1983) 197
Ab initio CI study of the photodissociation of nitrosyl chloride (ClNO), D. Solgadi, F. Lahmani, C. Lardeux and J.P. Flament 79 (1983) 225

Internal heavy-atom effect on the T_1 states of monochloroquinolines and monochloronaphthalenes, J. Najbar, W. Jarzeba and Z.H. Urbanek 79 (1983) 245
Angle-resolved photoelectron spectroscopy of the chloro-substituted methanes, P.R. Keller, J.W. Taylor, T.A. Carlson and F.A. Grimm 79 (1983) 269
Secondary amines: a low-temperature dielectric relaxation study, J. Gilchrist and H. Godfrin 79 (1983) 307
Argon ion laser excitation of supersonic seeded molecular beams of I_2, F.J. Aoiz, M.M. Oprysko and R.B. Bernstein 79 (1983) 321
Search for the laser-induced crossed beam reaction of excited I_2 ($B\,^3\Pi$) with Hg, M.M. Oprysko, F.J. Aoiz, R.B. Bernstein and M.A. McMahan 79 (1983) 341
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. II. Calculation of spin–orbit coupling, J. Baiardo and M. Vala 79 (1983) 403
Effective core potential calculations using frozen orbitals. Applications to transition metals, L.G.M. Pettersson, U. Wahlgren and O. Gropen 80 (1983) 7
Breakdown in the Koopmans' theorem interpretation of the outer valence-level photoemission spectra of selected organic molecules, R.W. Bigelow 80 (1983) 45
Primary amines: a low-temperature dielectric relaxation study, J. Gilchrist 80 (1983) 63
Photofragmentation of HI in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 80 (1983) 113
Vibrational effects with excitation transfer in metastable rare-gas–halide collisions, M.S. de Vries and R.M. Martin 80 (1983) 157
The effect of a magnetic field on discrete and continuum CS_2 fluorescence, S.J. Silvers, M.R. McKeever and G.K. Chawla 80 (1983) 177
Semiclassical calculation of energy transfer in polyatomic molecules. IX. Cross sections for $M + CO_2(000) \rightarrow M + CO_2(nml)$ (M = He and Ar), G.D. Billing and D.C. Clary 80 (1983) 213
Finite perturbation MCSCF and CI calculations of nuclear spin–spin coupling constants for some molecules with multiple bonds, A. Laaksonen, J. Kowalewski and V.R. Saunders 80 (1983) 221
Magnetic susceptibility of 1,1′,2,2′-tetramethylcobaltocene and 1,1′-diethylcobaltocene: evidence for the dynamic Jahn–Teller effect, E. König, V.P. Desai, B. Kanellakopulos and F.H. Köhler 80 (1983) 263
Determination of the dipole moment of thioformaldehyde in the $\tilde{a}\,^3A_2$ excited state by laser phosphorescence excitation spectroscopy, D.J. Clouthier and C.M.L. Kerr 80 (1983) 299
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. III. Single-crystal Zeeman spectroscopy, J. Baiardo, M. Vala and I. Trabjerg 80 (1983) 305
On the nature of the fluorescent state of methylated indole derivatives, S.R. Meech, D. Phillips and A.G. Lee 80 (1983) 317
Autoionization spectra of Li_2 and the $X\,^2\Sigma_g^+$ ground state of Li_2^+: experimental and theoretical investigations, D. Eisel, W. Demtröder, W. Müller and P. Botschwina 80 (1983) 329
Dissociative excitation of SiH_4, SiD_4, Si_2H_6 and GeH_4 by 0–100 eV electron impact, J. Perrin and J.F.M. Aarts 80 (1983) 351
Angular distribution for the major photoelectron bands of nitrogen below 45 eV binding energy, F.A. Grimm and Th.A. Carlson 80 (1983) 389

Free radicals
Theory of optically detected magnetic resonance spectra of radical pairs, A.B. Doktorov, O.A. Anisimov, A.I. Burshtein and Yu.N. Molin 71 (1982) 1
Rotational spectrum and hyperfine structure of the $^2\Sigma$ radicals BaF and BaCl, Ch. Ryzlewicz, H.-U. Schütze-Pahlmann, J. Hoeft and T. Törring 71 (1982) 389

α-hydroxyalkyl radicals by photoreduction in aprotic solvents: ESR spectra, ab initio potential function, inversion–internal rotation dynamics and temperature dependence of coupling constants of 1-hydroxyethyl, G. Cirelli, T.-K. Ha, R. Meyer and Hs.H. Günthard 72 (1982) 15
Emission and laser excitation spectra of rotationally cooled cations in the gas phase: $\tilde{A}\,^2\Pi \leftrightarrow \tilde{X}\,^2\Pi$ band systems of $H(C{\equiv}C)_2X^+$, X = Cl, Br, D. Klapstein, J.P. Maier, L. Misev and W. Zambach 72 (1982) 101
Unified theoretical treatment of analytic first and second energy derivatives in open-shell Hartree–Fock theory, Y. Osamura, Y. Yamaguchi, P. Saxe, M.A. Vincent, J.F. Gaw and H.F. Schaefer III 72 (1982) 131
Temperature dependence of the reactions of CH radicals with unsaturated hydrocarbons, M.R. Berman, J.W. Fleming, A.B. Harvey and M.C. Lin 73 (1982) 27
Muonium-substituted organic free radicals in liquids. Muon–electron hyperfine coupling constants and the selectivity of formation of methyl- and fluorine-substituted cyclohexadienyl-type radicals, E. Roduner, G.A. Brinkman and P.W.F. Louwrier 73 (1982) 117
An ab initio molecular orbital study of the ammonium radical, B.N. McMaster, J. Mrozek and V.H. Smith Jr. 73 (1982) 131
Ab initio calculations as first step towards the structure of free radicals. I. Geometries and energies of the ethyl analogs $NH_2CH_3^+$ and $CH_2NH_3^+$, L. Bonazzola, N. Leray and Y. Ellinger 73 (1982) 145
Temperature dependence of $C_3(X\,^1\Sigma_g^+)$ reactions with alkenes and alkynes, 295–610 K, H.H. Nelson, H. Helvajian, L. Pasternack and J.R. McDonald 73 (1982) 431
Energy-transfer reactions between $He(2\,^3S)$ and $Ne(^3P_{0,2})$ metastable atoms and PN radicals, H. Obase, M. Tsuji and Y. Nishimura 74 (1983) 89
Electron hopping and magnetic field dependent spin dynamics of radical ions in solution, H.W. Krüger, M.E. Michel-Beyerle and E.W. Knapp 74 (1983) 205
Excitation and emission spectra of the $^2A_2'' \leftrightarrow {}^2E_1''$ system of the gas-phase cyclopentadienyl radical, H.H. Nelson, L. Pasternack and J.R. McDonald 74 (1983) 227
Detection of transient laser magnetic resonance signals in pulsed CO_2 laser irradiation of SF_2/H_2O and SF_6/NO mixtures, J.S. Geiger, D.R. Smith and J.D. Bonnett 74 (1983) 239
Detection and identification of free radicals in the gaseous-phase ozonolysis of ethylene: microreactor–matrix ESR spectroscopy, F.J. Rákóczi, T.-K. Ha and Hs.H. Günthard 74 (1983) 273
Spectroscopic properties of the methyl radical calculated from UHF SCEP wavefunctions, P. Botschwina, J. Flesch and W. Meyer 74 (1983) 321
Kinetics of methyl radical reaction with methanol at 20–105 K, V.L. Vyazovkin, B.V. Bol'shakov and V.A. Tolkatchev 75 (1983) 11
Photoabsorption spectrum of radicals produced by a pulsed discharge of trace H_2O in Ar, R.L. Day and L.C. Lee 75 (1983) 17
The ESR spectrum of the C_5F_5 radical, T. Chen (Dschen), F. Graf and Hs.H. Günthard 75 (1983) 165
Analysis of restricted rotation of the acetyl group in *m*- and *p*-nitroacetophenone anion radicals, M. Branca, A. Gamba, C. Oliva and M. Simonetta 75 (1983) 253
Structure and photodecomposition reactions of cations of cyclopentane, cyclohexane, cyclic olefines and dienes in γ-irradiated frozen solutions of CF_3CCl_3. An ESR study, M. Tabata and A. Lund 75 (1983) 379
Intramolecular vibrational relaxation in the dual-channel 5-methyl-3-hexyl radical system excited by different activation pathways, S.P. Wrigley, K.W. Smith and B.S. Rabinovitch 75 (1983) 453
Experimental and theoretical study on cation radicals of cyclopropane, cyclobutane and cyclopentane, K. Ohta, H. Nakatsuji, H. Kubodera and T. Shida 76 (1983) 271

Theoretical approach to fluorine substitution in X_2NO and X_2CN free radicals. Comparison between ab initio UHF and RHF + perturbation treatments, V. Barone, F. Lelj, N. Russo, Y. Ellinger and R. Subra 76 (1983) 385
Electron spin echo decay kinetics of an ion track in β-irradiated frozen solution of sulfuric acid. Numerical simulation by the Monte Carlo method and experiment, A.M. Raitsimring and V.V. Tregub 77 (1983) 123
Ab initio study of the thermodynamic and kinetic stability of the ammonium radical, H. Cardy, D. Liotard, A. Dargelos and E. Poquet 77 (1983) 287
The nascent translational energy of difluorocarbene produced in IR MPD of the penta-fluoroethyl radical, D.M. Rayner, S. Kimel and P.A. Hackett 77 (1983) 349
The kinetics of the retarded reaction of free radicals with oxygen in a methanol glass, V.A. Bagryansky, V.M. Zaskul'nikov and V.A. Tolkatchev 78 (1983) 41
Photolytic production of $O(^3P)$ in the presence of CF_3I: the formation of $IF(X\,^1\Sigma^+)$, T.A. Watson, M. Addison and C. Wittig 78 (1983) 57
Magnetic field effects on the recombination of radical ions in reaction centers of photo-synthetic bacteria, W. Lersch and M.E. Michel-Beyerle 78 (1983) 115
Emission spectra of supersonically cooled methyldiacetylene cations, S. Leutwyler, D. Klapstein and J.P. Maier 78 (1983) 151
The $B\,^2\Sigma^+$–$X\,^2\Sigma^+$ system of SrF: precise spectroscopic constants from a combined fit of microwave and sub-Doppler optical spectra, W.E. Ernst and J.O. Schröder 78 (1983) 363
Kinetic studies of the bromine–oxygen system: a new paramagnetic particle, BrO_2, N.I. Butkovskaya, I.I. Morozov, V.L. Tal'rose and E.S. Vasiliev 79 (1983) 21
Flash photolysis electron spin resonance and CIDEP studies of radicals derived from nitrogen heterocyclics. I. The diazanaphthalenes, S. Basu, K.A. McLauchlan and A.J.D. Ritchie 79 (1983) 95
Can the H_5 molecule be observed?, K. Kaufmann, M. Jungen and V. Staemmler 79 (1983) 111
Formation of $NH(A\,^3\Pi, c\,^1\Pi)$ by electron-impact dissociation of HN_3, I. Tokue and Y. Ito 79 (1983) 383
Rotational perturbations in the CN $(B\,^2\Sigma^+$–$X\,^2\Sigma^+)$ tail band system. I. Analysis of the $v = 27$ and 30 levels of $CN(A\,^2\Pi_i)$, Y. Ozaki, T. Nagata, K. Suzuki, T. Kondow and K. Kuchitsu 80 (1983) 73
Rotational perturbation in the $CN(B\,^2\Sigma^+$–$X\,^2\Sigma^+)$ tail band system. II. Identification of the $CN(^4\Pi)$ state and its vibrational levels, Y. Ozaki, H. Ito, K. Suzuki, T. Kondow and K. Kuchitsu 80 (1983) 85
Radiative lifetime and quenching of $SO(b\,^1\Sigma^+, v' = 0)$, J. Wildt, E.H. Fink, R. Winter and F. Zabel 80 (1983) 167
Determination of rate constants for some reactions of CBr radicals by VUV laser flash photolysis, L. Hellner, K.T.V. Grattan and M.H.R. Hutchinson 80 (1983) 345
Dissociative excitation of SiH_4, SiD_4, Si_2H_6 and GeH_4 by 0–100 eV electron impact, J. Perrin and J.F.M. Aarts 80 (1983) 351

Excitons
Photochemical control of energy transfer in molecular crystals, J.S. Patel and D.M. Hanson 72 (1982) 35
The motion of triplet excitons in β-phase crystals of 9,10-dichloroanthracene, R. Krauss, W. Schrof, H.C. Wolf and D. Schmid 73 (1982) 55
Charge-transfer transitions in crystalline anthracene and their role in photoconductivity, L. Sebastian, G. Weiser, G. Peter and H. Bässler 75 (1983) 103
A model of localization, soliton propagation, and self-trapping in an electronically excited atomic lattice, M.A. Collins and D.P. Craig 75 (1983) 191

Comparative reinvestigation of the interaction of phonons with Wannier and Frenkel excitons in crystalline solids, J. Singh 75 (1983) 371
Delayed-fluorescence ODMR and EPR studies of triplet excitons in charge-transfer molecular crystals, G. Agostini, C. Corvaja, G. Giacometti and L. Pasimeni 77 (1983) 233
Dynamics of energy transport in ternary molecular solids. II. Time evolution of naphthalene fluorescence, P. Argyrakis and R. Kopelman 78 (1983) 251
On the use of X-ray-excited optical luminescence (XEOL) for the analysis of multisite rare-earth systems, P. Tola, A. Retournard, J. Dexpert-Ghys, M. Lemonnier, M. Pagel and J. Goulon 78 (1983) 339
Triplet-state optical spectra of highly concentrated isotopically mixed crystals of anthracene A-h_{10}:A-d_{10}, D. Rund and H. Port 78 (1983) 357
Dispersive singlet exciton motion in an organic glass, R. Jankowiak and H. Bässler 79 (1983) 57
Polarization energy of a localized charge in a molecular crystal. VI. Effect of excitons, I. Eisenstein and R.W. Munn 79 (1983) 189
Theory of coherence effects in time-delayed fluorescence. II. Application to two- and three-dimensional crystals, A. Fort, V. Ern and V.M. Kenkre 80 (1983) 205
Singlet exciton migration in a random organic two-component system containing physical and chemical traps, G. Peter, B. Ries and H. Bässler 80 (1983) 289

Defects and impurities
X-ray structure and optical properties of silver films prepared by condensation of preformed Ag-clusters, W. Vogel, B. Tesche and W. Schulze 74 (1983) 137
Electrostatic energy of vacancy formation in crystals of polar molecules, R.W. Munn 74 (1983) 301
Polarization energy of a localized charge in a molecular crystal. IV. Effect of polarizability changes, I. Eisenstein, R.W. Munn and P.J. Bounds 74 (1983) 307
Are new chemical species in anthracene crystals formed as a result of charge-carrier trapping at physical defects?, Z. Zboiński 75 (1983) 297
Some problems of recombination kinetics. I, E. Kotomin and V. Kuzovkov 76 (1983) 479
Polarization energy of a localized charge in a molecular crystal. V. Effect of vacancies, I. Eisenstein and R.W. Munn 77 (1983) 47
Dependence of photochemical and photophysical hole burning on laser intensity, A.U. Jalmukhambetov and I.S. Osad'ko 77 (1983) 247
On the use of X-ray-excited optical luminescence (XEOL) for the analysis of multisite rare-earth systems, P. Tola, A. Retournard, J. Dexpert-Ghys, M. Lemonnier, M. Pagel and J. Goulon 78 (1983) 339
Charge transfer in polar media. Transition-state entropy, Yu.I. Dakhovskii and A.A. Ovchinnikov 80 (1983) 17
On the role of the dynamic Jahn–Teller effect in the spectra of matrix-isolated atoms with strong spin–orbit coupling, C.M. Weinert, F. Forstmann, R. Grinter and D.M. Kolb 80 (1983) 95

Ions and complexes
Electron affinities of higher molybdenum fluorides as determined by the effusion technique, L.N. Sidorov, A.Ya. Borshchevsky, E.B. Rudny and V.D. Butsky 71 (1982) 145
C-13 magnetic relaxation rates and H-1 and C-13 paramagnetic shifts of Ni(II) complex of dopamine, A. Lai, M. Monduzzi, G. Saba, M. Casu and G. Crisponi 71 (1982) 271
A semiclassical model for the vibrational excitation of spherical-top molecules in collisions with ions, T. Ellenbroek and J.P. Toennies 71 (1982) 309

Unimolecular dissociations of excited $C_3H_6O^+$: a comparative photoelectron–photoion coincidence study of 1,2-epoxypropane and acetone, R. Bombach, J.-P. Stadelmann and J. Vogt 72 (1982) 259
A study of picosecond dehalogenation of chlorobenzene anions in liquids by positronium inhibition measurements, G. Wikander and O.E. Mogensen 72 (1982) 407
Ab initio calculations of radiative transition probabilities in the $X\,^1\Sigma^+$ state SiO and the $X\,^2\Sigma^+$ and $A\,^2\Pi$ states of SiO^+, H.-J. Werner, P. Rosmus and M. Grimm 73 (1982) 169
Limited configuration interaction calculation of the optical spectrum for the permanganate ion, H. Johansen and S. Rettrup 74 (1983) 77
High-resolution spectroscopy of N_2O^+ in the near ultraviolet using FIBLAS (fast-ion-beam laser spectroscopy), S. Abed, M. Broyer, M. Carré, M.L. Gaillard and M. Larzillière 74 (1983) 97
A theoretical study of the condensation reactions of methyl cation with ammonia, water, hydrogen fluoride and hydrogen sulphide, R.H. Nobes and L. Radom 74 (1983) 163
Anomalous rotational distributions in electronic emission of supersonically cooled H_2O^+ ($\widetilde{A}\,^2A_1 \rightarrow \widetilde{X}\,^2B_1$), S. Leutwyler, D. Klapstein and J.P. Maier 74 (1983) 441
Benchmark measurement of iodobenzene ion fragmentation rates, J. Dannacher, H.M. Rosenstock, R. Buff, A.C. Parr, R.L. Stockbauer, R. Bombach and J.-P. Stadelmann 75 (1983) 23
The electronic structure of chalcogen hexahalogenides, G.L. Gutsev and A.P. Klyagina 75 (1983) 243
Analysis of restricted rotation of the acetyl group in *m*- and *p*-nitroacetophenone anion radicals, M. Branca, A. Gamba, C. Oliva and M. Simonetta 75 (1983) 253
Unusual low-energy isomers for simple radical cations, M.J. Frisch, K. Raghavachari, J.A. Pople, W.J. Bouma and L. Radom 75 (1983) 323
Internal energy dependence of the autodetachment and dissociation times of the SF_6^- ion, J.P. Astruc, R. Barbé, A. Lagrèze and J.P. Schermann 75 (1983) 405
Fractionally charged ions in crystal lattices of organic ion-radical salts, L. Komorowski 76 (1983) 31
A model for the interpretation of the electronic spectra of the complex ions $M(bpy)_3^{2+}$ (M = Fe, Ru, Os) in D_3 and C_2 sites, J. Ferguson and F. Herren 76 (1983) 45
Studies of some iron dithiolate complexes by the ESCA, Mössbauer and extended Hückel methods, J. Blomquist, U. Helgeson, B. Folkesson and R. Larsson 76 (1983) 71
Kinetic energy release distribution in the fragmentation of energy-selected iodopropane ions, W.A. Brand, T. Baer and C.E. Klots 76 (1983) 111
Intensities in inelastic neutron scattering spectra: a test of recent theory, J. Howard, B.C. Boland and J. Tomkinson 77 (1983) 145
An NMR relaxation study of hydrogen exchange and its deuterium isotope effects in aqueous carboxylic acid solutions, D. Lankhorst, J. Schriever and J.C. Leyte 77 (1983) 319
Charge transfer to a solvent state. VIII. Localization of charge during the transition state of the solute: the solute cation localization energy, T.B. Truong 77 (1983) 377
Emission spectra of rotationally cooled dihaloacetylene cations in the gas phase: $\widetilde{A}\,^2\Pi_{\Omega,g} \rightarrow \widetilde{X}\,^2\Pi_{\Omega,u}$ band systems, D. Klapstein, J.P. Maier and W. Zambach 77 (1983) 463
Mössbauer spectroscopic study of the electronic and magnetic properties of iron(II) para-toluenesulphonate, J.S. Haynes, A.R. Hume, J.R. Sams and R.C. Thompson 78 (1983) 127
Emission spectra of supersonically cooled dimethyldiacetylene cations, D. Klapstein, R. Kuhn, S. Leutwyler and J.P. Maier 78 (1983) 167
Interaction potentials for Li^+–rare-gas systems, L.A. Viehland 78 (1983) 279
Bifurcation diagrams for two substrate oscillatory systems, J. Maselko 78 (1983) 381
Classical treatment of a Heisenberg linear chain with spin alternation; application to the $MnNi(EDAT)\cdot 6H_2O$ complex, M. Drillon, E. Coronado, D. Beltran and R. Georges 79 (1983) 449
Charge transfer in polar media. Transition-state entropy, Yu.I. Dakhnovskii and A.A. Ovchinnikov 80 (1983) 17

The theory of transitions between electronic states. Application to radiationless transitions in polar solvents, L.D. Zusman 80 (1983) 29
Comment on "Scaling relationship in photoelectron–photoion coincidence studies: the acetone ion dissociation", D.J. McAdoo 80 (1983) 203
Theoretical study on the structure and stability of hydrogen-ion clusters H_n^+ and H_n^- (n = 3,5,7,11,13), K. Hirao and S. Yamabe 80 (1983) 237
Infrared-enhanced multiphoton dissociation of iodobenzene cations, N.B. Lev and R.C. Dunbar 80 (1983) 367

Dimers and molecular clusters

The bond nature of alkaline-earth homonuclear metal clusters investigated with pseudopotential CI method, G. Pacchioni and J. Koutecký 71 (1982) 181
The direct reaction field hamiltonian: analysis of the dispersion term and application to the water dimer, B.T. Thole and P.Th. van Duijnen 71 (1982) 211
Evidence for the existence of structure in gas-phase homomolecular clusters of water, V. Herman, B.D. Kay and A.W. Castleman Jr. 72 (1982) 185
Polymerization of TS-12 diacetylene crystals: crystal structure of monomer and polymer and spectroscopy of reaction intermediates, D. Siegel, H. Sixl, V. Enkelmann and G. Wenz 72 (1982) 201
Relativistically parameterized extended Hückel calculations. VII. Nuclear spin–spin coupling tensors and densities of states for cluster models of CdTe, HgTe and PbTe, A. Viste, M. Hotokka, L. Laaksonen and P. Pyykkö 72 (1982) 225
Influence of the molecular environment in solution measurements of the second-order optical susceptibility for urea and derivatives, I. Ledoux and J. Zyss 73 (1982) 203
Some observations on molecular complexes of carbon monoxide in argon and oxygen matrices, M. Diem, T.-L. Tso and E.K.C. Lee 73 (1982) 283
Photoelectron spectroscopic study of simple hydrogen-bonded dimers. I. Supersonic nozzle beam photoelectron spectrometer and the formic-acid dimer, S. Tomoda, Y. Achiba, K. Nomoto, K. Sato and K. Kimura 74 (1983) 113
Photoelectron spectroscopic study of simple hydrogen-bonded dimers. II. The methanol dimer, S. Tomoda and K. Kimura 74 (1983) 121
The rotational spectrum and molecular properties of a hydrogen-bonded dimer of phosphine and hydrogen fluoride, A.C. Legon and L.C. Willoughby 74 (1983) 127
A model for two-electron four-center mixed valence systems. Applications to $[W_4O_8Cl_8(H_2O)_4]^{2-}$, J.J. Girerd and J.P. Launay 74 (1983) 217
A combination of pseudopotentials and density functionals: results for Li_n^{m+}, Na_n^{m+} and K_n^{m+} clusters ($n \leqslant 4$; m = 0,1), J. Flad, G. Igel, M. Dolg, H. Stoll and H. Preuss 75 (1983) 331
Calculated ro-vibrational fine-structure spectrum and weak-field Zeeman splittings of the O_2Ar van der Waals molecule, J. Tennyson and J. Mettes 76 (1983) 195
Electric dipole moments of $(HC^{15}N)_2$ and $HC^{15}NH^{35}Cl$, E.J. Campbell and S.G. Kukolich 76 (1983) 225
An extended Hückel study of hydrogen and oxygen chemisorption on Ru(001) surface, B.C. Khanra and S.K. Saha 76 (1983) 255
Fermi resonance and bandshapes in deuterated palmitic acid, P. Piaggio, G. Dellepiane, R. Tubino and L. Piseri 77 (1983) 185
Long-range interactions of Li(n = 2) states with each other and the long-range interaction of Li(2s ^{2}S) with Li(3s ^{2}S), D.D. Konowalow and J.L. Fish 77 (1983) 435
Photodissociation of molecular beams of N_2O_4, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 78 (1983) 65

The effect of molecular excitation on crystal packing. 9-cyano- and 9,10-dimethylanthracene as excited guest/host and host/guest pairs, K. Norris, P. Gray, D.P. Craig, C.P. Mallett and B.R. Markey 79 (1983) 9
Collisional and radiational energy transfer in the system $Na^*(3\,^2P) + Na_2(X\,^1\Sigma^+) \rightarrow Na(3\,^2S) + Na_2^*(A\,^1\Sigma^+)$, P. Arrowsmith, S.H.P. Bly, P.E. Charters, P. Chevrier, J.C. Polanyi and H.H. Telle 79 (1983) 31
Ab initio studies on hydrogen-bonded chains. III. The linear, infinite chain of hydrogen cyanide molecules, A. Karpfen 79 (1983) 211
Temperature dependence of J-band aggregate of the dye 1,1′-diethyl-2,2′-cyanine bromide studied by steady-state and time-resolved picosecond fluorescence spectroscopy, Z.X. Yu, P.Y. Lu and R.R. Alfano 79 (1983) 289
Electronic spectroscopy of fluorobenzene van der Waals molecules by resonant two-photon ionization, K. Rademann, B. Brutschy and H. Baumgärtel 80 (1983) 129
Vibrational predissociation of van der Waals clusters of ethylene, G. Fischer, R.E. Miller and R.O. Watts 80 (1983) 147
Theoretical study on the structure and stability of hydrogen-ion clusters H_n^+ and H_n^- (n = 3,5,7,9,11,13), K. Hirao and S. Yamabe 80 (1983) 237
Conformational energetics in hydrogen-bonded dimers. The unobserved CO–HF complex, M.A. Benzel and C.E. Dykstra 80 (1983) 273
Matrix-isolation spectroscopy of Pb_2, H. Sontag, B. Eberle and R. Weber 80 (1983) 279

Polymers and biological macromolecules

The fluctuating-force formulation of friction drag coefficients, J.M. Schurr 71 (1982) 101
Studies of oriented Langmuir–Blodgett multilayers by infrared linear dichroism, P.-A. Chollet and J. Messier 73 (1982) 235
Non-hydrodynamic contribution to the concentration dependence of the self diffusion of interacting brownian macroparticles, G.D.J. Phillies 74 (1983) 197
A crystal orbital investigation on the one-dimensional bis(glyoximato)pyrazine–iron system, M.C. Böhm 76 (1983) 1
Resonance Raman scattering and absorption spectroscopy of substituted polyenes, J. Berréhar, C. Lapersonne-Meyer, M. Schott and M. le Postollec 77 (1983) 11
Theory of sorption of gases on polymers. II. Effects of inter-chain secondary bonds, M. Pyda and M. Kurzyński 79 (1983) 219
Quasi-elastic light scattering studies on T7 DNA in the presence of a sinusoidal electric field, K.S. Schmitz 79 (1983) 297
Classical treatment of a Heisenberg linear chain with spin alternation; application to the $MnNi(EDTA)\cdot 6H_2O$ complex, M. Drillon, E. Coronado, D. Beltran and R. Georges 79 (1983) 449
A theoretical estimate for quasihomopolar singlet levels in long polyenes with a spin model hamiltonian, K. Hashimoto 80 (1983) 253

PHENOMENA

Atomic and molecular structure

Conformational interconversions in supersonic jets: matrix IR spectroscopy and model calculations, P. Felder and Hs.H. Günthard 71 (1982) 9
Are atoms intrinsic to molecular electronic wavefunctions? I. The FORS model, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 41
Are atoms intrinsic to molecular electronic wavefunctions? II. Analysis of FORS orbitals, K. Ruedenberg, M.W. Schmidt and M.M. Gilbert 71 (1982) 51

Are atoms intrinsic to molecular electronic wavefunctions? III. Analysis of FORS configurations, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 65
Ab initio calculation of the zero-field splittings of the $X\,^3\Sigma_g^-$ and $B\,^3\Pi_{g,i}$ states of the S_2 molecule, B.A. Hess, R.J. Buenker, C.M. Marian and S.D. Peyerimhoff 71 (1982) 79
Features of the photochemically active state surfaces of azobenzene, S. Monti, G. Orlandi and P. Palmieri 71 (1982) 87
The selection of coordinate systems for describing large-amplitude nuclear motion in triatomic molecules, R. Wallace 71 (1982) 173
The bond nature of alkaline-earth homonuclear metal clusters investigated with pseudo-potential CI method, G. Pacchioni and J. Koutecký 71 (1982) 181
Electronic properties by Green's function calculations. Renormalized optical potential results: Ne, Ar, HF, H_2O, NH_3, I. Cacelli, R. Moccia and V. Carravetta 71 (1982) 199
Inelastic neutron scattering study of low frequency motions in $[Co(C_5H_5)_2^+]$ and $[Cr(C_6H_6)_2^+]$ intercalated in the $MnPS_3$ layered compound, C. Sourisseau, Y. Mathey and C. Poinsignon 71 (1982) 257
Dynamic polarizability of many-electron systems within a time-dependent density-functional theory, S.K. Ghosh and B.M. Deb 71 (1982) 295
On the use of "effective harmonic potentials" and "effective normal coordinates" in computing the vibrational energy levels of polyatomic molecules, G. Amat 71 (1982) 363
Rotational spectrum and hyperfine structure of the $^2\Sigma$ radicals BaF and BaCl, Ch. Ryzlewicz, H.-U. Schütze-Pahlmann, J. Hoeft and T. Törring 71 (1982) 389
Avoided-crossing molecular-beam spectroscopy of CH_3SiF_3, W.L. Meerts and I. Ozier 71 (1982) 401
Superfine and hyperfine structure in the ν_3 band of $^{32}SF_6$, J. Bordé and Ch.J. Bordé 71 (1982) 417
Highly resolved optical spectra of *o*-durylene, W.P. Cofino, G.Ph. Hoornweg, C. Gooijer, C. MacLean and N.H. Velthorst 72 (1982) 73
Inequivalent methyl CH oscillators in methyl-substituted conjugated compounds as revealed by higher overtone spectra, R. Nakagaki and I. Hanazaki 72 (1982) 93
Emission and laser excitation spectra of rotationally cooled cations in the gas phase: $\widetilde{A}\,^2\Pi \leftrightarrow \widetilde{X}\,^2\Pi$ band systems of $H(C{\equiv}C)_2X^+$, X = Cl, Br, D. Klapstein, J.P. Maier, L. Misev and W. Zambach 72 (1982) 101
Potential energy curves and transition moments for the low-lying electronic states of the Si_2 molecule, S.D. Peyerimhoff and R.J. Buenker 72 (1982) 111
Unified theoretical treatment of analytic first and second energy derivatives in open-shell Hartree–Fock theory, Y. Osamura, Y. Yamaguchi, P. Saxe, M.A. Vincent, J.F. Gaw and H.F. Schaefer III 72 (1982) 131
A spin-adapted linear response theory in a coupled-cluster framework for direct calculation of spin-allowed and spin-forbidden transition energies, S. Ghosh, D. Mukherjee and S.N. Bhattacharyya 72 (1982) 161
The structure of F_2O_2: theoretical predictions and comparisons with F_2 and F_2O, R. Ahlrichs and P.R. Taylor 72 (1982) 287
Phonon spectra and structure of crystalline ethylene oxide and ethylene sulphide at 77 K, R. Cataliotti and G. Paliani 72 (1982) 293
Ab initio study on cyanamide and isocyanamide, K. Ichikawa, Y. Hamada, Y. Sugawara, M. Tsuboi, S. Kato and K. Morokuma 72 (1982) 301
Studies using the CASSCF wavefunction, P.J. Knowles, G.J. Sexton and N.C. Handy 72 (1982) 337
Theoretical studies of the electronic spectrum of thioformaldehyde, P.G. Burton, S.D. Peyerimhoff and R.J. Buenker 73 (1982) 83

Muonium-substituted organic free radicals in liquids. Muon–electron hyperfine coupling constants and the selectivity of formation of methyl- and fluorine-substituted cyclohexadienyl-type radicals, E. Roduner, G.A. Brinkman and P.W.F. Louwrier 73 (1982) 117
An ab initio molecular orbital study of the ammonium radical, B.N. McMaster, J. Mrozek and V.H. Smith Jr. 73 (1982) 131
Ab initio calculations as first step towards the structure of free radicals. I. Geometries and energies of the ethyl analogs $NH_2CH_3^+$ and $CH_2NH_3^+$, L. Bonazzola, N. Leray and Y. Ellinger 73 (1982) 145
An ab initio study of relationships between bond lengths and the harmonic and anharmonic cross-coupling constants involving the double bonds in hetero-atom substituted conjugated dienes, C.W. Bock, M. Trachtman and P. George 73 (1982) 179
Influence of the oxy, aza and thio groups on the electron affinities of carbonyl compounds studied by means of ETS, A. Modelli, G. Distefano and D. Jones 73 (1982) 395
Photochemical decay of butynal ($H_3CC{\equiv}C{-}CHO$) in the gas phase following $S_1(n\pi^*) \leftarrow S_0$ excitation, H.U. Zürcher, U. Brühlmann and J.R. Huber 73 (1982) 403
Calculation of the ^{14}N and ^2H quadrupole coupling tensor in trimeric inidazole, M.H. Palmer, F.E. Scott and J.A.S. Smith 74 (1983) 9
The polarization dependence of two-photon absorption rates for randomly oriented molecules, M.A.C. Nascimento 74 (1983) 51
Molecular translational–rovibronic hamiltonian. I. Non-linear molecules, R. Islampour and M. Kasha 74 (1983) 67
High-resolution spectroscopy of N_2O^+ in the near ultraviolet using FIBLAS (fast-ion-beam laser spectroscopy), S. Abed, M. Broyer, M. Carré, M.L. Gaillard and M. Larzillière 74 (1983) 97
The rotational spectrum and molecular properties of a hydrogen-bonded dimer of phosphine and hydrogen fluoride, A.C. Legon and L.C. Willoughby 74 (1983) 127
A theoretical study of the condensation reactions of methyl cation with ammonia, water, hydrogen fluoride and hydrogen sulphide, R.H. Nobes and L. Radom 74 (1983) 163
Excitation and emission spectra of the $^2A_2'' \leftrightarrow {}^2E_1''$ system of the gas-phase cyclopentadienyl radical, H.H. Nelson, L. Pasternack and J.R. McDonald 74 (1983) 227
Angle-resolved photoelectron measurements on the 2p orbitals of Si in SiF_4 and $Si(CH_3)_4$ in the gas phase, P.R. Keller, J.W. Taylor, F.A. Grimm, P. Senn, T.A. Carlson and M.O. Krause 74 (1983) 247
Spectroscopic properties of the methyl radical calculated from UHF SCEP wavefunctions, P. Botschwina, J. Flesch and W. Meyer 74 (1983) 321
Theoretical solvent effects on molecular structure and spectroscopic properties through the virtual-charge model. Application to the inverted solvatochromy of benzophenone $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ absorption bands, A. Botrel, F. Corre and A. le Beuze 74 (1983) 383
Convergence of an improved CIPS algorithm, S. Evangelisti, J.-P. Daudey and J.P. Malrieu 75 (1983) 91
Resonant non-linear spectroscopy in strong fields, B. Dick and R.M. Hochstrasser 75 (1983) 133
Molecular translational–rovibronic hamiltonian. II. Linear molecules, R. Islampour and M. Kasha 75 (1983) 157
The electronic structure of chalcogen hexahalogenides, G.L. Gutsev and A.P. Klyagina 75 (1983) 243
High-resolution HeI and HeII photoelectron spectra of the zinc and cadmium dihalide valence bands, D.J. Bristow, G.W. Bancroft and J.S. Tse 75 (1983) 263
High-resolution HeI and HeII photoelectron spectra of the Zn 3d and Cd 4d orbitals in the zinc and cadmium dihalides: ligand field splittings and intensity variations, G.M. Bancroft, D.J. Bristow and J.S. Tse 75 (1983) 277
Unusual low-energy isomers for simple radical cations, M.J. Frisch, K. Raghavachari, J.A. Pople, W.J. Bouma and L. Radom 75 (1983) 323

A combination of pseudopotentials and density functionals: results for Li_n^{m+}, Na_n^{m+} and K_n^{m+} clusters ($n \leqslant 4$; $m = 0,1$), J. Flad, G. Igel, M. Dolg, H. Stoll and H. Preuss 75 (1983) 331
Structure and photodecomposition reactions of cations of cyclopentane, cyclohexane, cyclic olefines and dienes in γ-irradiated frozen solutions of CF_3CCl_3. An ESR study, M. Tabata and A. Lund 75 (1983) 379
Molecular structure and photoelectron spectra of H_2S, H_2Se, and H_2Te. Effective core potential calculations on ground and valence ionic states, J. Müller, L.J. Sæthre and O. Gropen 75 (1983) 395
Cluster expansion of the wavefunction. Valence and Rydberg excitations, ionizations, and inner-valence ionizations of CO_2 and N_2O studied by the SAC and SAC CI theories, H. Nakatsuji 75 (1983) 425
A model for the interpretation of the electronic spectra of the complex ions $M(bpy)_3^{2+}$ (M = Fe, Ru, Os) in D_3 and C_2 sites, J. Ferguson and F. Herren 76 (1983) 45
Studies of some iron dithiolate complexes by the ESCA, Mössbauer and extended Hückel methods, J. Blomquist, U. Helgeson, B. Folkesson and R. Larsson 76 (1983) 71
Molecular orbital electron momentum distributions and separation energies of CH_3CN, A. Minchinton, C.E. Brion, J.P.D. Cook and E. Weigold 76 (1983) 89
Density functional estimates of charge transfer and chemical potentials in hydrogen halides and mixed halides, J.A. Alonso and N.H. March 76 (1983) 121
Vibrational energy disposal in reactions of fluorine atoms with hydrides of groups III, IV and V, A.S. Manocha, D.W. Setser and M.A. Wickramaaratchi 76 (1983) 129
The radiative lifetime of the $A\,^1\Pi$ state of CH^+ calculated from long CAS SCF expansions, M. Larsson and P.E.M. Siegbahn 76 (1983) 175
MS Xα and LCAO Xα calculations of ionization potentials. A comparison with Koopmans' theorem and accurate calculations, G. de Alti, P. Decleva and A. Lisini 76 (1983) 185
Calculated ro-vibrational fine-structure spectrum and weak-field Zeeman splittings of the O_2Ar van der Waals molecule, J. Tennyson and J. Mettes 76 (1983) 195
Experimental and theoretical study on cation radicals of cyclopropane, cyclobutane and cyclopentane, K. Ohta, H. Nakatsuji, H. Kubodera and T. Shida 76 (1983) 271
Spectroscopic investigation of the electronic structure of the chlorine molecule in the VUV, Th. Moeller, B. Jordan, P. Gürtler, G. Zimmerer, D. Haaks, J. le Calve and M.C. Castex 76 (1983) 295
Study of the dependence of spin–orbit matrix elements on AO basis set composition for inner and valence shells: results for the multiplet splitting of $X\,^3\Sigma^-$ and $C\,^3\Pi$ of SO and $X\,^2\Pi$ in SO^+, R. Klotz, C.M. Marian, S.D. Peyerimhoff, B.A. Hess and R.J. Buenker 76 (1983) 367
Theoretical approach to fluorine substitution in X_2NO and X_2CN free radicals. Comparison between ab initio UHF and RHF + perturbation treatments, V. Barone, F. Lelj, N. Russo, Y. Ellinger and R. Subra 76 (1983) 385
The N1s shake-up spectrum of para-aminobenzonitrile. A theoretical and experimental ESCA study, P.-Å. Malmquist, S. Svensson and H. Ågren 76 (1983) 429
Infrared-induced conformational isomerization of ethylene glycol in a low-temperature argon matrix, H. Takeuchi and M. Tasumi 77 (1983) 21
Relaxation and spectroscopy of CaCl in seeded supersonic beams, U. Buck, J. Kesper, H.H. Kuge and D. Otten 77 (1983) 201
The role of tautomeric and rotameric species in the photophysics of 2-(2′-hydroxyphenyl)-benzoxazole, G.J. Woolfe, M. Melzig, S. Schneider and F. Dörr 77 (1983) 213
Oscillator strengths and lifetimes of the $C_2\,A\,^1\Pi_u - X\,^1\Sigma_g^+$ Phillips system, E.F. van Dishoeck 77 (1983) 277
Ab initio study of the thermodynamic and kinetic stability of the ammonium radical, H. Cardy, D. Liotard, A. Dargelos and E. Poquet 77 (1983) 287

Longe-range interactions of Li(n = 2) states with each other and the long-range interaction of Li(2s ^{2}S) with Li(3s ^{2}S), D.D. Konowalow and J.L. Fish 77 (1983) 435
Structure and properties of a model of deoxyheme. An ab initio SCF calculation, M.-M. Rohmer, A. Dedieu and A. Veillard 77 (1983) 449
Emission spectra of rotationally cooled dihaloacetylene cations in the gas phase: $\tilde{A}\,^2\Pi_{\Omega,g} \rightarrow \tilde{X}\,^2\Pi_{\Omega,u}$ band systems, D. Klapstein, J.P. Maier and W. Zambach 77 (1983) 463
Theoretical three-dimensional potential-energy surface for the reaction of Be with HF, S. Chapman, M. Dupuis and S. Green 78 (1983) 93
Proper characterization of MC SCF stationary points, J.T. Golab, D.L. Yeager and P. Jørgensen 78 (1983) 175
Complete valence-shell ionization spectra of N_2 and CO: application of the extended two-particle–hole Tamm–Dancoff approximation (2ph-TDA), J. Schirmer and O. Walter 78 (1983) 201
High-resolution UV photoelectron spectrum of CO_2, I. Reineck, C. Nohre, R. Maripuu, P. Lodin, S.H. Al-Shamma, H. Veenhuizen, L. Karlsson and K. Siegbahn 78 (1983) 311
On the use of X-ray-excited optical luminescence (XEOL) for the analysis of multisite rare-earth systems, P. Tola, A. Retournard, J. Dexpert-Ghys, M. Lemonnier, M. Pagel and J. Goulon 78 (1983) 339
On a site-selective EXAFS experiment using optical emission, J. Goulon, P. Tola, M. Lemonnier and J. Dexpert-Ghys 78 (1983) 347
The B $^2\Sigma^+$–X $^2\Sigma^+$ system of SrF: precise spectroscopic constants from a combined fit of microwave and sub-Doppler optical spectra, W.E. Ernst and J.O. Schröder 78 (1983) 363
Valence-shell photoabsorption by CO_2 and its connections with electron–CO_2 scattering, P.M. Dittman, D. Dill and J.L. Dehmer 78 (1983) 405
Angle-resolved photoelectron spectroscopy of the chloro-substituted methanes, P.R. Keller, J.W. Taylor, T.A. Carlson and F.A. Grimm 79 (1983) 269
Time-reversal symmetry, Kramers' degeneracy and the algebraic eigenvalue problem, N. Rösch 80 (1983) 1
Rotational perturbations in the CN (B $^2\Sigma^+$–X $^2\Sigma^+$) tail band system. I. Analysis of the v = 27 and 30 levels of CN (A $^2\Pi_i$), Y. Ozaki, T. Nagata, K. Suzuki, T. Kondow and K. Kuchitsu 80 (1983) 73
Rotational perturbation in the CN (B $^2\Sigma^+$–X $^2\Sigma^+$) tail band system. II. Identification of the CN ($^4\Pi$) state and its vibrational levels, Y. Ozaki, H. Ito, K. Suzuki, T. Kondow and K. Kuchitsu 80 (1983) 85
Photofragmentation of HI in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 80 (1983) 113
Theoretical study of shake-up in the core photoelectron spectra of the alkali atoms, G. de Alti, P. Decleva and A. Lisini 80 (1983) 229
Theoretical study on the structure and stability of hydrogen-ion clusters H_n^+ and H_n^- (n = 3,5,7,9,11,13), K. Hirao and S. Yamabe 80 (1983) 237
Conformational energetics in hydrogen-bonded dimers. The unobserved CO–HF complex, M.A. Benzel and C.E. Dykstra 80 (1983) 273
Matrix-isolation spectroscopy of Pb_2, H. Sontag, B. Eberle and R. Weber 80 (1983) 279
Determination of the dipole moment of thioformaldehyde in the $\tilde{a}\,^3A_2$ excited state by laser phosphorescence excitation spectroscopy, D.J. Clouthier and C.M.L. Kerr 80 (1983) 299

Energy levels

Are atoms intrinsic to molecular electronic wavefunctions? I. The FORS model, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 41
Are atoms intrinsic to molecular electronic wavefunctions? II. Analysis of FORS orbitals, K. Ruedenberg, M.W. Schmidt and M.M. Gilbert 71 (1982) 51

Are atoms intrinsic to molecular electronic wavefunctions? III. Analysis of FORS configurations, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 65
Ab initio calculation of the zero-field splittings of the $X\,^3\Sigma_g^-$ and $B\,^3\Pi_{g,i}$ states of the S_2 molecule, B.A. Hess, R.J. Buenker, C.M. Marian and S.D. Peyerimhoff 71 (1982) 79
The selection of coordinate systems for describing large-amplitude nuclear motion in triatomic molecules, R. Wallace 71 (1982) 173
Fermi-coupled spherically adapted effective states in the collisionless multiphoton excitation of SF_6, C. di Lauro and F. Lattanzi 71 (1982) 233
Synchrotron-radiation photoemission study of the V–VI layered compounds Bi_2Te_3, Bi_2Se_3, Sb_2Te_3 and Sb_2Te_2Se, M.R. Thuler, R.L. Benbow and Z. Hurych 71 (1982) 265
On the use of "effective harmonic potentials" and "effective normal coordinates" in computing the vibrational energy levels of polyatomic molecules, G. Amat 71 (1982) 363
The vibrational energy manifold of the lowest lying bending mode of tricarbon oxide sulfide, O=C=C=C=S, as determined by relate intensity measurements, M. Winnewisser and E.W. Peau 71 (1982) 377
Rotational spectrum and hyperfine structure of the $^2\Sigma$ radicals BaF and BaCl, Ch. Ryzlewicz, H.-U. Schütze-Pahlmann, J. Hoeft and T. Törring 71 (1982) 389
α-hydroxyalkyl radicals by photoreduction in aprotic solvents: ESR spectra, ab initio potential function, inversion–internal rotation dynamics and temperature dependence of coupling constants of 1-hydroxyethyl, G. Cirelli, T.-K. Ha, R. Meyer and Hs.H. Günthard 72 (1982) 15
X-ray photoemission and optical spectra of $NiPS_3$, $FePS_3$ and $ZnPS_3$, M. Piacentini, F.S. Khumalo, G. Leveque, C.G. Olson and D.W. Lynch 72 (1982) 61
Low-temperature vibronic spectra of 1,1′-binaphthyl, M.J. Riley, A.R. Lacey, M.G. Sceats and R.G. Gilbert 72 (1982) 83
Potential energy curves and transition moments for the low-lying electronic states of the Si_2 molecule, S.D. Peyerimhoff and R.J. Buenker 72 (1982) 111
Atoms-in-molecules calculations on diatomic fragments of polyatomic systems: HeH, HeH^+ and HeH^- for a DIM model of Penning ionization of H_2 by He*, I. Paidarová, J. Vojtík and R. Polák 72 (1982) 119
A spin-adapted linear response theory in a coupled-cluster framework for direct calculation of spin-allowed and spin-forbidden transition energies, S. Ghosh, D. Mukherjee and S.N. Bhattacharyya 72 (1982) 161
Relativistically parameterized extended Hückel calculations. VII. Nuclear spin–spin coupling tensors and densities of states for cluster models of CdTe, HgTe and PbTe, A. Viste, M. Hotokka, L. Laaksonen and P. Pyykkö 72 (1982) 225
Photoelectron spectra and their relativistic interpretation for gaseous bismuth trihalides, R.G. Egdell, M. Hotokka, L. Laaksonen, P. Pyykkö and J.G. Snijders 72 (1982) 237
Studies using the CASSCF wavefunction, P.J. Knowles, G.J. Sexton and N.C. Handy 72 (1982) 337
Electronic–vibrational excitation of a hydrogen-bonded molecule in supersonic expansions: 1,4-dihydroxyanthraquinone and its deuterated derivatives, G. Smulevich, A. Amirav, U. Even and J. Jortner 73 (1982) 1
Satellites in the X-ray photoelectron spectra of transition-metal and rare-earth compounds, D.D. Sarma, P. Vishnu Kamath and C.N.R. Rao 73 (1982) 71
An ab initio molecular orbital study of the ammonium radical, B.N. McMaster, J. Mrozek and V.H. Smith Jr. 73 (1982) 131
Autoionization in HCl and DCl by photoelectron spectroscopy, P. Natalis, P. Pennetreau, L. Longton and J.E. Collin 73 (1982) 191
Stimulated Raman investigation of CO_2-laser-excited SF_6, P. Esherick, A.J. Grimley and A. Owyoung 73 (1982) 271

Influence of the oxy, aza and thio groups on the electron affinities of carbonyl compounds studied by means of ETS, A. Modelli, G. Distefano and D. Jones 73 (1982) 395
High-resolution absorption spectra of diphenylmethylenes, D.J. Graham and T.-S. Lin 73 (1982) 411
The dual phosphorescence of benzophenazine in ethanol, G.W. Suter and U.P. Wild 73 (1982) 421
Calculation of the ^{14}N and ^{2}H quadrupole coupling tensor in trimeric imidazole, M.H. Palmer, F.E. Scott and J.A.S. Smith 74 (1983) 9
Limited configuration interaction calculation of the optical spectrum for the permanganate ion, H. Johansen and S. Rettrup 74 (1983) 77
Photoelectron spectroscopic study of simple hydrogen-bonded dimers. I. Supersonic nozzle beam photoelectron spectrometer and the formic-acid dimer, S. Tomoda, Y. Achiba, K. Nomoto, K. Sato and K. Kimura 74 (1983) 113
Photoelectron spectroscopic study of simple hydrogen-bonded dimers. II. The methanol dimer, S. Tomoda and K. Kimura 74 (1983) 121
A model for two-electron four-center mixed valence systems. Applications to $[W_4O_8Cl_8(H_2O)_4]^{2-}$, J.J. Girerd and J.P. Launay 74 (1983) 217
Excitation and emission spectra of the $^{2}A_2'' \leftrightarrow {}^{2}E_1''$ system of the gas-phase cyclopentadienyl radical, H.H. Nelson, L. Pasternack and J.R. McDonald 74 (1983) 227
Spectroscopic properties of the methyl radical calculated from UHF SCEP wavefunctions, P.Botschwina, J. Flesch and W. Meyer 74 (1983) 321
Large-amplitude vibration in triatoms. II. Introduction of potential refinement within a LAV model applied to the sulfur dioxide molecule, R. Wallace 74 (1983) 339
Jahn–Teller splitting of the 3s → 3p transition of sodium isolated in a xenon matrix, J. Hormes and J. Schiller 74 (1983) 433
Electronic structure of potassium clusters (K_9, K_{15}, K_{27}) by the SCF Xα(LSD) SW method, A. Pellegatti, B.N. McMaster and D.R. Salahub 75 (1983) 83
Charge-transfer transitions in crystalline anthracene and their role in photoconductivity, L. Sebastian, G. Weiser, G. Peter and H. Bässler 75 (1983) 103
Fluorescence from the a ^{5}P and a ^{3}P states of matrix-isolated Fe atoms, M.T. McKenzie Jr. and E.R. Nixon 75 (1983) 115
Molecular translational–rovibronic hamiltonian. II. Linear molecules, R. Islampour and M. Kasha 75 (1983) 157
The semiclassical determination of potential surfaces from observed spectra. I, S.M. Colwell and I.C. Percival 75 (1983) 215
The semiclassical determination of potential surfaces from observed spectra. II, S.M. Colwell and I.C. Percival 75 (1983) 225
High-resolution HeI and HeII photoelectron spectra of the zinc and cadmium dihalide valence bands, D.J. Bristow, G.M. Bancroft and J.S. Tse 75 (1983) 263
High-resolution HeI and HeII photoelectron spectra of the Zn 3d and Cd 4d orbitals in the zinc and cadmium dihalides: ligand field splittings and intensity variations, G.M. Bancroft, D.J. Bristow and J.S. Tse 75 (1983) 277
A crystal orbital investigation on the one-dimensional bis(glyoximato)pyrazine iron system, M.C. Böhm 76 (1983) 1
Vibrational energy disposal in reactions of fluorine atoms with hydrides of groups III, IV and V, A.S. Manocha, D.W. Setser and M.A. Wickramaaratchi 76 (1983) 129
Double-ionization Auger satellites obtained by the Green's function method, C.-M. Liegener 76 (1983) 397
Large-amplitude vibration in triatoms. III. Application to linear molecules: vibrational states of HCN, R. Wallace 76 (1983) 421
A XANES study of mixed-valence transition-metal oxides and rare-earth alloys, G. Sankar, P.R. Sarode and C.N.R. Rao 76 (1983) 435

Resonance Raman scattering and absorption spectroscopy of substituted polyenes, J. Berréhar, C. Lapersonne-Meyer, M. Schott and M. le Postollec 77 (1983) 11
The nature of the stabilizing effect of thio groups on the Π anion states of benzene studied by means of electron transmission spectroscopy, A. Modelli, D. Jones, F.P. Colonna and G. Distefano 77 (1983) 153
Spectroscopic studies of the photochromism of N-salicylideneaniline mixed crystals and glasses, D. Higelin and H. Sixl 77 (1983) 391
Atoms-in-molecules study of ground- and excited-state potential-energy curves for Li_2, R. Polák and J. Vojtík 78 (1983) 107
Emission spectra of supersonically cooled methyldiacetylene cations, S. Leutwyler, D. Klapstein and J.P. Maier 78 (1983) 151
Emission spectra of supersonically cooled dimethyldiacetylene cations, D. Klapstein, R. Kuhn, S. Leutwyler and J.P. Maier 78 (1983) 167
The $B\,^2\Sigma^+ - X\,^2\Sigma^+$ system of SrF: precise spectroscopic constants from a combined fit of microwave and sub-Doppler optical spectra, W.E. Ernst and J.O. Schröder 78 (1983) 363
Flash photolysis electron spin resonance and CIDEP studies of radicals derived from nitrogen heterocyclics. I. The diazanaphthalenes, S. Basu, K.A. McLauchlan and A.J.D. Ritchie 79 (1983) 95
Ab initio CI study of the photodissociation of nitrosyl chloride (ClNO), D. Solgadi, F. Lahmani, C. Lardeux and J.P. Flament 79 (1983) 225
Spectroscopic properties of Er^{3+} ions in Li(Er,Gs) P_4O_{12} single crystals – fluorescence, Raman and infrared spectra, Z. Mazurak, J. Hanuza, K. Hermanowicz, B. Jeżowska-Trzebiatowska, D. Schultze and Ch. Waligora 79 (1983) 255
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. I. Single-crystal polarized absorption spectrum, J. Baiardo, M. Vala and I. Trabjerg 79 (1983) 391
A new approach to the determination of good action–angle variables for coupled oscillator systems, L.C. Geiger and G.C. Schatz 79 (1983) 431
Rotational perturbations in the CN ($B\,^2\Sigma^+ - X\,^2\Sigma^+$) tail band system. I. Analysis of the $v = 27$ and 30 levels of CN ($A\,^2\Pi_i$), Y. Ozaki, T. Nagata, K. Suzuki, T. Kondow and K. Kuchitsu 80 (1983) 73
Rotational perturbations in the CN ($B\,^2\Sigma^+ - X\,^2\Sigma^+$) tail band system. II. Identification of the CN ($^4\Pi$) state and its vibrational levels, Y. Ozaki, H. Ito, K. Suzuki, T. Kondow and K. Kuchitsu 80 (1983) 85
New I_2 emission from iodine atom recombination reaction, K.-H. Stephan-Rossbach and F.J. Comes 80 (1983) 121
Electronic spectroscopy of fluorobenzene van der Waals molecules by resonant two-photon ionization, K. Rademann, B. Brutschy and H. Baumgärtel 80 (1983) 129
Theoretical study of shake-up in the core photoelectron spectra of the alkali atoms, G. de Alti, P. Decleva and A. Lisini 80 (1983) 229
A theoretical estimate for quasihomopolar singlet levels in long polyenes with a spin model hamiltonian, K. Hashimoto 80 (1983) 253
Matrix-isolation spectroscopy of Pb_2, H. Sontag, B. Eberle and R. Weber 80 (1983) 279
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. III. Single-crystal Zeeman spectroscopy, J. Baiardo, M. Vala and I. Trabjerg 80 (1983) 305

Electric and magnetic properties

Near-degeneracy effects and efficiency of MBPT calculations of molecular properties. Polarizability curve of H_2, G.H.F. Diercksen, M. Jaszuński and A.J. Sadlej 71 (1982) 105

Dynamic polarizability of many-electron systems within a time-dependent density-functional theory, S.K. Ghosh and B.M. Deb 71 (1982) 295
Ab initio calculation of the equilibrium geometry and the ^{13}C, ^{17}O and ^{27}Al NMR chemical shielding tensors of the system Al^{3+}/CO, Th. Weller, W. Meiler, A. Michael, H.J. Köhler, H. Lischka and R. Höller 72 (1982) 155
Studies of magnetic field effects on the intensity and the lifetime of sulfur dioxide luminescence in the gas phase, V.I. Makarov, N.L. Lavrik and N.M. Bazhin 72 (1982) 213
Relativistically parameterized extended Hückel calculations. VII. Nuclear spin–spin coupling tensors and densities of states for cluster models of CdTe, HgTe and PbTe, A. Viste, M. Hotokka, L. Laaksonen and P. Pyykkö 72 (1982) 225
Studies using the CASSCF wavefunction, P.J. Knowles, G.J. Sexton and N.C. Handy 72 (1982) 337
Diamagnetic anisotropy of molecular complexes of 1,3,5-trinitrobenzene with anthracene and carbazole, R. Burzyński and T. Luty 72 (1982) 441
Ab initio calculations of radiative transition probabilities in the $X\,^1\Sigma^+$ state of SiO and the $X\,^2\Sigma^+$ and $A\,^2\Pi$ states of SiO^+, H.-J. Werner, P. Rosmus and M. Grimm 73 (1982) 169
Magnetic resonance experiments on the radical cation salt $(fluoranthenyl)_2^+PF_6^-$. Correlation of proton-NMR, fluorine-NMR and ESR, W. Höptner, M. Mehring, J.U. von Schütz, H.C. Wolf, B.S. Morra, V. Enkelmann and G. Wegner 73 (1982) 253
On the relativistic theory of NMR chemical shifts, P. Pyykkö 74 (1983) 1
Calculation of the ^{14}N and ^2H quadrupole coupling tensor in trimeric imidazole, M.H. Palmer, F.E. Scott and J.A.S. Smith 74 (1983) 9
Polarization energy of a localized charge in a molecular crystal. IV. Effect of polarizability changes, I. Eisenstein, R.W. Munn and P.J. Bounds 74 (1983) 307
The dipole moment of ^7LiH and ^7LiD in the excited $A^1\Sigma^+$ state: a test of the Born–Oppenheimer approximation, M. Brieger, A. Renn, A. Sodeik and A. Hese 75 (1983) 1
Electronic structure of potassium clusters (K_9, K_{15}, K_{27}) by the SCF Xα(LSD) SW method, A. Pellegatti, B.N. McMaster and D.R. Salahub 75 (1983) 83
Charge-transfer transitions in crystalline anthracene and their role in photoconductivity, L. Sebastian, G. Weiser, G. Peter and H. Bässler 75 (1983) 103
The ESR spectrum of the C_5F_5 radical, T. Chen (Dschen), F. Graf and Hs.H. Günthard 75 (1983) 165
Are new chemical species in anthracene crystals formed as a result of charge-carrier trapping at physical defects?, Z. Zboiński 75 (1983) 297
Measurement of the ^{14}N nuclear quadrupole couplings in the lowest ($n\pi^*$) excited triplet state of pyrazine by ODMR, W. Fröhling, C.J. Winscom and K. Möbius 75 (1983) 389
Ionization potentials and polarization energies of tetraselenafulvalene (TSF) derivatives determined from ultraviolet photoelectron spectroscopy, N. Sato, G. Saito and H. Inokuchi 76 (1983) 79
Electric dipole moments of $(HC^{15}N)_2$ and $HC^{15}NH^{35}Cl$, E.J. Campbell and S.G. Kukolich 76 (1983) 225
Unified theory of the electronic Stark effect in molecular crystals, R.W. Munn 76 (1983) 243
Experimental and theoretical study on cation radicals of cyclopropane, cyclobutane and cyclopentane, K. Ohta, H. Nakatsuji, H. Kubodera and T. Shida 76 (1983) 271
Theoretical approach to fluorine substitution in X_2NO and X_2CN free radicals. Comparison between ab initio UHF and RHF + perturbation treatments, V. Barone, F. Lelj, N. Russo, Y. Ellinger and R. Subra 76 (1983) 385
Solvent effects on the potential energy surfaces of molecular iodine: a spectroscopic study, M. Geilhaupt and Th. Dorfmüller 76 (1983) 443
Polarization energy of a localized charge in a molecular crystal. V. Effect of vacancies, I. Eisenstein and R.W. Munn 77 (1983) 47

Perturbation theory of the electron correlation effects for atomic and molecular properties. VI. Complete active space (CAS) SCF and MBPT calculations of electric properties of the FH molecule, G.H.F. Diercksen, V. Kellö, B.O. Roos and A.J. Sadlej 77 (1983) 93
Finite-field many-body perturbation theory. VI. Multipole polarizabilities of beryllium. A comparative study, G.H.F. Diercksen and A.J. Sadlej 77 (1983) 429
Magnetic field effects on the recombination of radical ions in reaction centers of photosynthetic bacteria, W. Lersch and M.E. Michel-Beyerle 78 (1983) 115
Mössbauer spectroscopic study of the electronic and magnetic properties of iron(II) paratoluenesulphonate, J.S. Haynes, A.R. Hume, J.R. Sams and R.C. Thompson 78 (1983) 127
Hartree–Fock–Slater LCAO calculation of the Mössbauer parameters of some antimony compounds, W. Ravenek, J.W.M. Jacobs and A. van der Avoird 78 (1983) 391
Measurements of depolarization ratios of gaseous linear chain molecules: a test of the principle of the additivity of bond polarizabilities, J.E.M. Haverkort, F. Baas and J.J.M. Beenakker 79 (1983) 105
Polarization energy of a localized charge in a molecular crystal. VI. Effect of excitons, I. Eisenstein and R.W. Munn 79 (1983) 189
Classical treatment of a Heisenberg linear chain with spin alternation; application to the MnNi(EDTA)·$6H_2O$ complex, M. Drillon, E. Coronado, D. Beltran and R. Georges 79 (1983) 449
The effect of a magnetic field on discrete and continuum CS_2 fluorescence, S.J. Silvers, M.R. McKeever and G.K. Chawla 80 (1983) 177
Finite perturbation MCSCF and CI calculations of nuclear spin–spin coupling constants for some molecules with multiple bonds, A. Laaksonen, J. Kowalewski and V.R. Saunders 80 (1983) 221
Magnetic susceptibility of 1,1′,2,2′-tetramethylcobaltocene and 1,1′-diethylcobaltocene: evidence for the dynamic Jahn–Teller effect, E. König, V.P. Desai, B. Kanellakopulos and F.H. Köhler 80 (1983) 263
Determination of the dipole moment of thioformaldehyde in the $\tilde{a}\ ^3A_2$ excited state by laser phosphorescence excitation spectroscopy, D.J. Clouthier and C.M.L. Kerr 80 (1983) 299

Spectral bandshapes and intensities

Theory of optically detected magnetic resonance spectra of radical pairs, A.B. Doktorov, O.A. Anisimov, A.I. Burshtein and Yu.N. Molin 71 (1982) 1
Absorption spectra of volatile aromatic hydrocarbon films in the vacuum ultraviolet region, S. Hino, T. Veszprémi, K. Ohno, H. Imokuchi and K. Seki 71 (1982) 135
The vibrational energy manifold of the lowest lying bending mode of tricarbon oxide sulfide, O=C=C=C=S, as determined by relative intensity measurements, M. Winnewisser and E.W. Peau 71 (1982) 377
Time-resolved spectroscopy: wavepacket formalism in the coherent-state representation, A.A. Villaeys and K.F. Freed 72 (1982) 1
Highly resolved optical spectra of *o*-durylene, W.P. Cofino, G.Ph. Hoornweg, C. Gooijer, C. MacLean and N.H. Velthorst 72 (1982) 73
Low-temperature vibronic spectra of 1,1′-binaphthyl, M.J. Riley, A.R. Lacey, M.G. Sceats and R.G. Gilbert 72 (1982) 83
Computer simulation of dichloromethane. II. Molecular dynamics, M. Ferrario and M.W. Evans 72 (1982) 147
A new extended diffusion model for rotational motion of symmetric-top molecules in the liquid phase, J. Lascombe, M. Besnard and P. Maraval 72 (1982) 177
Two-photon excitations of bond modes, M.L. Sage and J. Jortner 72 (1982) 249

Random coupling models. IV. Numerical investigation of the dependence on the random coupling distribution and on the initial phases, B. Carmeli, R. Tulman, A. Nitzan and M.H. Kalos 72 (1982) 363
Pulse substructure in passively and synchronously mode-locked cw dye lasers, D.P. Millar and A.H. Zewail 72 (1982) 381
Ab initio calculations of radiative transition probabilities in the $X\,^1\Sigma^+$ state of SiO and the $X\,^2\Sigma^+$ and $A\,^2\Pi$ states of SiO^+, H.-J. Werner, P. Rosmus and M. Grimm 73 (1982) 169
Vibrational relaxation of hydrogen-bonded species in solution. IV. Temperature and concontration dependence of the ν_σ(OH---N) band of phenol–pyridine, U.P. Agarwal, R.S. Green and J. Yarwood 74 (1983) 35
Non-hydrodynamic contribution to the concentration dependence of the self diffusion of interaction brownian macroparticles, G.D.J. Phillies 74 (1983) 197
Absolute dipole oscillator strengths for molecular and dissociative photoionization of hydrogen fluoride, F. Carnovale and C.E. Brion 74 (1983) 253
Theoretical model for calculations of infrared and Raman band profiles of strong hydrogen bonds in ordered media, F. Fillaux 74 (1983) 395
Calculations of infrared and Raman band profiles of strong hydrogen bonds. OH stretching bands and proton dynamics in crystalline potassium hydrogen carbonate, F. Fillaux 74 (1983) 405
Anomalous rotational distributions in electronic emission of supersonically cooled H_2O^+ ($\tilde{A}\,^2A_1 \rightarrow \tilde{X}\,^2B_1$), S. Leutwyler, D. Klapstein and J.P. Maier 74 (1983) 441
Photoabsorption spectrum of radicals produced by a pulsed discharge of trace H_2O in Ar, R.L. Day and L.C. Lee 75 (1983) 17
Classical aspects of the laser excitation of a Morse oscillator, S.K. Gray 75 (1983) 67
Fluorescence from the $a\,^5P$ and $a\,^3P$ states of matrix-isolated Fe atoms, M.T. McKenzie Jr. and E.R. Nixon 75 (1983) 115
Two-frequency CO_2 laser multiple-photon dissociation and dynamics of excited state absorption in CDF_3, I.P. Herman 75 (1983) 121
Resonant non-linear spectroscopy in strong fields, B. Dick and R.M. Hochstrasser 75 (1983) 133
Analysis of restricted rotation of the acetyl group in *m*- and *p*-nitroacetophenone anion radicals, M. Branca, A. Gamba, C. Oliva and M. Simonetta 75 (1983) 253
Comparative reinvestigation of the interaction of phonons with Wannier and Frenkel excitons in crystalline solids, J. Singh 75 (1983) 371
Cluster expansion of the wavefunction. Valence and Rydberg excitations, ionizations, and inner-valence ionizations of CO_2 and N_2O studied by the SAC and SAC CI theories, H. Nakatsuji 75 (1983) 425
Binary theory of dephasing in liquid solutions. I. The non-markovian theory of encounters, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 149
Binary theory of dephasing in liquid solutions. II. Motion-transformed isotropic Raman spectra, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 163
The radiative lifetime of the $A\,^1\Pi$ state of CH^+ calculated from long CAS SCF expansions, M. Larsson and P.E.M. Siegbahn 76 (1983) 175
Cluster expansion of the wavefunction. Outer- and inner-valence ionization spectra of CS_2 and COS, H. Nakatsuji 76 (1983) 283
Double-ionization Auger satellites obtained by the Green's function method, C.-M. Liegener 76 (1983) 397
Space- and time-resolved resonance-enhanced vibrational Raman spectroscopy from a femtosecond-lived singlet excited state of β-carotene, L.V. Haley and J.A. Koningstein 77 (1983) 1
Vibronic and multimode effects on the Raman excitation profile of a totally symmetric fundamental in the Soret band of cytochrome **c**, W. Siebrand and M.Z. Zgierski 77 (1983) 35

Theoretical analysis of photoelectron angular distributions of linear molecules, W. Thiel 77 (1983) 103
Intensities in inelastic neutron scattering spectra: a test of recent theory, J. Howard, B.C. Boland and J. Tomkinson 77 (1983) 145
Fermi resonance and bandshapes in deuterated palmitic acid, P. Piaggio, G. Dellepiane, R. Tubino and L. Piseri 77 (1983) 185
Oscillator strengths and lifetimes of the C_2 $A\,^1\Pi_u$–$X\,^1\Sigma_g^+$ Phillips system, E.F. van Dishoeck 77 (1983) 277
Ultrafast non-radiative decay via conical intersections of molecular potential-energy surfaces: $C_2H_4^+$, H. Köppel 77 (1983) 359
Raman spectroscopic studies on the dynamics of a molecular "probe" (methyl iodide) in hydrocarbon solvents, W.F. Pacynko, J. Yarwood and D.J. Gardiner 78 (1983) 319
Triplet-state optical spectra of highly concentrated isotopically mixed crystals of anthracene A-h_{10}: A-d_{10}, D. Rund and H. Port 78 (1983) 357
Collisional and radiational energy transfer in the system $Na^*(3\,^2P) + Na_2(X\,^1\Sigma^+) \rightarrow NA(3\,^2S) + Na_2^*(A\,^1\Sigma^+)$, P. Arrowsmith, S.H.P. Bly, P.E. Charters, P. Chevrier, J.C. Polanyi and H.H. Telle 79 (1983) 31
A quantitative analysis of the ν_s(IR) bands of H-bonds. I. Theory, Y. Marechal 79 (1983) 69
A quantitative analysis of the ν_s(IR) bands of H-bonds. II. Adipic acid crystals, Y. Marechal 79 (1983) 85
Shape resonances and the photodissociation cross section of MgH near threshold, S.S. Bhattacharyya and D. Basu 79 (1983) 129
Argon ion laser excitation of supersonic seeded molecular beams of I_2, F.J. Aoiz, M.M. Oprysko and R.B. Bernstein 79 (1983) 321
Fluorescence lifetime and collisional quenching of the predissociative NO $B\,^2\Pi(v' = 7)$ state, K. Shibuya and F. Stuhl 79 (1983) 367
The lowest triplet state of tetramethyl-1,3-cyclobutanedithione. II. Calculation of spin–orbit coupling, J. Baiardo and M. Vala 79 (1983) 403
Breakdown in the Koopmans' theorem interpretation of the outer valence-level photoemission spectra of selected organic molecules, R.W. Bigelow 80 (1983) 45
On the role of the dynamic Jahn–Teller effect in the spectra of matrix-isolated atoms with strong spin–spin coupling, C.M. Weinert, F. Forstmann, R. Grinter and D.M. Kolb 80 (1983) 95
Vibrational predissociation of van der Waals clusters of ethylene, G. Fisher, R.E. Miller and R.O. Watts 80 (1983) 147
Comparison of photon-stimulated dissociation of gas-phase, solid and chemisorbed water, D.E. Ramaker 80 (1983) 183

Relaxation phenomena

On the use of laser-induced fluorescence to study free-jet expansions, P. Willems, H. Hulsman and F. Aerts 71 (1982) 27
The fluctuating-force formulation of friction drag coefficients, J.M. Schurr 71 (1982) 101
C-13 magnetic relaxation rates and H-1 and C-13 paramagnetic shifts of Ni(II) complex of dopamine, A. Lai, M. Monduzzi, G. Saba, M. Casu and G. Crisponi 71 (1982) 271
Collision transfers between CdH $A\,^2\Pi\ v' = 0$ rotational states induced by He or Ar, J. Dufayard and O. Nedelec 71 (1982) 279
Photon echoes stimulated from long-lived ordered populations in multi-level systems. The effect of intersystem crossing and optical branching, J.B.W. Morsink, W.H. Hesselink and D.A. Wiersma 71 (1982) 289
Intense shake-up satellites in the XPS spectra of planar and sterically hindered N-piperidyl-nitrobenzenes and -nitrothiophens, G. Distefano, M. Guerra, F.P. Colonna, D. Jones, G. Consiglio and D. Spinelli 72 (1982) 267

Raman scattering study of toluene vibrational relaxation in benzene–toluene liquid system, W. Reimschüssel, H. Abramczyk, H. Barańska and A. Łabudzinska 72 (1982) 313
Random coupling models. IV. Numerical investigation of the dependence on the random coupling distribution and on the initial phases, B. Carmeli, R. Tulman, A. Nitzan and M.H. Kalos 72 (1982) 363
Pulse substructure in passively and synchronously mode-locked cw dye lasers, D.P. Millar and A.H. Zewail 72 (1982) 381
On the connection between incubation and relaxation times in thermal unimolecular reactions, H.O. Pritchard and S.R. Vatsya 72 (1982) 447
Electronic–vibrational excitations of a hydrogen-bonded molecule in supersonic expansions: 1,4-dihydroxyanthraquinone and its deuterated derivatives, G. Smulevich, A. Amirav, U. Even and J. Jortner 73 (1982) 1
Photon-induced molecular charge separation studied by nanosecond time-resolved microwave conductivity, M.P. de Haas and J.M. Warman 73 (1982) 35
Satellites in the X-ray photoelectron spectra of transition-metal and rare-earth compounds, D.D. Sarma, P. Vishnu Kamath and C.N.R. Rao 73 (1982) 71
Picosecond study of pinacyanol photophysics, J.C. Mialocq 73 (1982) 107
Magnetic resonance experiments on the radical cation salt (fluoranthenyl)$_2^+PF_6^-$. Correlation of proton-NMR, fluorine-NMR and ESR, W. Höptner, M. Mehring, J.U. von Schütz, H.C. Wolf, B.S. Morra, V. Enkelmann and G. Wegner 73 (1982) 253
Stimulated Raman investigation of CO_2-laser-excited SF_6, P. Esherick, A.J. Grimley and A. Owyoung 73 (1982) 271
Photodissociation of molecular beams of SO_2 at 193 nm, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 73 (1982) 377
Picosecond kinetics of radiationless relaxations of triphenyl methane dyes. Evidence for rapid excited-state equilibrium between states of differing geometry, V. Sundström, T. Gillbro and H. Bergström 73 (1982) 439
Relaxation of the individual vibrational levels of carbon monoxide following shock heating at 2100 K, J.P. Martin, M.R. Buckingham, J.A. Chenery and C.J.S.M. Simpson 74 (1983) 15
Vibrational relaxation of hydrogen-bonded species in solution. IV. Temperature and concentration dependence of the ν_σ(OH---N) band of phenol–pyridine, U.P. Agarwal, R.S. Green and J. Yarwood 74 (1983) 35
Vibrational relaxation times in polyatomic gas mixtures: on the validity of the linear mixture rule, Y.V. Chalapati Rao and B.V. Mallu 74 (1983) 43
Spectra and emission lifetimes of $H_2CS(\tilde{A}\,^1A_2)$, M. Kawasaki, K. Kasatani, Y. Ogawa and H. Sato 74 (1983) 83
Anharmonic processes in molecular crystals. Calculation of the anharmonic shifts, bandwidth and energy decay processes in crystalline naphthalene, R.G. Della Valle, P.F. Fracassi, R. Righini and S. Califano 74 (1983) 179
Detection of transient laser magnetic resonance signals in pulsed CO_2 laser irradiation of SF_6/H_2O and SF_6/NO mixtures, J.S. Geiger, D.R. Smith and J.D. Bonnett 74 (1983) 239
Vibrational relaxation of $CO_2(00^01)$ and $N_2O(00^01)$ by NO, F. Al Adel, L. Doyennette, M. Margottin-Maclou and L. Henry 74 (1983) 413
Anomalous rotational distributions in electronic emission of supersonically cooled H_2O^+ $(\tilde{A}\,^2A_1 \rightarrow \tilde{X}\,^2B_1)$, S. Leutwyler, D. Klapstein and J.P. Maier 74 (1983) 441
Acoustic study of a critical binary mixture of nitrobenzene and *n*-hexane at low and ultrasonic frequencies, H. Tanaka, Y. Wada and H. Nakajima 75 (1983) 37
Resonant non-linear spectroscopy in strong fields, B. Dick and R.M. Hochstrasser 75 (1983) 133

Vibrationally excited molecules and mechanisms of chemical and physical processes in non-equilibrium plasmas, P.A. Sergeev and D.I. Slovetsky 75 (1983) 231
Analysis of restricted rotation of the acetyl group in *m*- and *p*-nitroacetophenone anion radicals, M. Branca, A. Gamba, C. Oliva and M. Simonetta 74 (1983) 253
Nickel porphyrin photophysics and photochemistry. A picosecond investigation of ligand binding and release in the excited state, D. Kim, C. Kirmaier and D. Holten 75 (1983) 305
Intramolecular vibrational relaxation in the dual-channel 5-methyl-3-hexyl radical system excited by different activation pathways, S.P. Wrigley, K.W. Smith and B.S. Rabinovitch 75 (1983) 453
On the statistics of an ensemble of oscillators under excitation. IV. Evaluation of the time for kinetic excitation into the quasicontinuum based on Kramers' theory, V.N. Sazonov and I.E. Khromov 76 (1983) 25
Binary theory of dephasing in liquid solutions. I. The non-markovian theory of encounters, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 149
Comment on collisionless vibrational relaxation, W. Fuss 76 (1983) 343
Electron spin echo decay kinetics of an ion track in β-irradiated frozen solution of sulfuric acid. Numerical simulation by the Monte Carlo method and experiment, A.M. Raitsimring and V.V. Tregub 77 (1983) 123
Electronic spectra of jet-cooled azulene, M. Fujii, T. Ebata, N. Mikami and M. Ito 77 (1983) 191
Relaxation and spectroscopy of CaCl in seeded supersonic beams, U. Buck, J. Kesper, H.H. Kuge and D. Otten 77 (1983) 201
The role of tautomeric and rotameric species in the photophysics of 2-(2′-hydroxyphenyl)-benzoxazole, G.J. Woolfe, M. Melzig, S. Schneider and F. Dörr 77 (1983) 213
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. I. Ferroelectric behaviour, H.A. Kołodziej and S. Sorriso 77 (1983) 341
The nascent translational energy of difluorocarbene produced in IR MPD of the penta-fluoroethyl radical, D.M. Rayner, S. Kimel and P.A. Hackett 77 (1983) 349
Ultrafast non-radiative decay via conical intersections of molecular potential-energy surfaces: $C_2H_4^+$, H. Köppel 77 (1983) 359
Eigenvalues of the Boltzmann collision operator for binary gases: relaxation of anisotropic distributions, B. Shizgal and R. Blackmore 77 (1983) 417
The kinetics of the retarded reaction of free radicals with oxygen in a methanol glass, V.A. Bagryansky, V.M. Zaskul'nikov and V.A. Tokatchev 78 (1983) 41
Driven-echo and rotary-echo measurements of the spin coherence in triplet-state benzo-phenone, R. Gillies and A.M. Ponte Goncalves 78 (1983) 49
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. II. Isotopic effect, H.A. Kołodziej and S. Sorriso 78 (1983) 75
He–HF vibrational inelasticity at low and intermediate energies from quantum collision theory, F.A. Gianturco, U.T. Lamanna and G. Petrella 78 (1983) 81
Semiclassical theory of predissociation induced by rotational (Coriolis) coupling, H. Nakamura 78 (1983) 235
Non-Condon scheme of radiationless transitions for the Morse oscillator model, A.L. Sobolewski 78 (1983) 265
Raman spectroscopic studies on the dynamics of a molecular "probe" (methyl iodide) in hydrocarbon solvents, W.F. Pacynko, J. Yarwood and D.J. Gardiner 78 (1983) 319
Comparisons between experimental argon and Lennard-Jones 12:6 shear viscosities, D. Fincham and D.M. Heyes 78 (1983) 425
Viscosity dependence of internal conversion rates of polyatomic molecules, K.-E. Süsse, D.-G. Welsch and I. Madzgalla 78 (1983) 443

Collision dominated relaxation of electrons in a weakly ionized nitrogen plasma after abrupt change of the electric field, M. Capitelli, C. Gorse, J. Wilhelm and R. Winkler 79 (1983) 1
On the theory of adiabatic electron-transfer reactions in polar solvents, A.B. Helman 79 (1983) 235
Internal heavy-atom effect on the T_1 states of monochloroquinolines and monochloronaphthalenes, J. Najbar, W. Jarzeba and Z.H. Urbanek 79 (1983) 245
Temperature dependence of J-band aggregate of the dye 1,1′-diethyl-2,2′-cyanine bromide studied by steady-state and time-resolved picosecond fluorescence spectroscopy, Z.X. Yu, P.Y. Lu and R.R. Alfano 79 (1983) 289
Quasi-elastic light scattering studies on T7 DNA in the presence of a sinusoidal electric field, K.S. Schmitz 79 (1983) 297
Secondary amines: a low-temperature dielectric relaxation study, J. Gilchrist and H. Godfrin 79 (1983) 307
Vibrational energy relaxation of highly compressed gaseous H_2 and N_2, M. Châtelet, J. Kieffer and B. Oksengorn 79 (1983) 413
Dipole–phonon coupling and dielectric relaxation, R. Nigmatullin and L.A. Dissado 79 (1983) 455
Primary amines: a low-temperature dielectric relaxation study, J. Gilchrist 80 (1983) 63
Vibrational predissociation of van der Waals clusters of ethylene, G. Fischer, R.E. Miller and R.O. Watts 80 (1983) 147
Comment on "Scaling relationships in photoelectron–photoion coincidence studies: the acetone ion dissociation", D.J. McAdoo 80 (1983) 203
On the nature of the fluorescent state of methylated indole derivatives, S.R. Meech, D. Phillips and A.G. Lee 80 (1983) 317
Intensity dependence of CO_2-laser-induced multiphoton absorption and decomposition of monomethylamine, D.K. Evans, R.D. McAlpine, H.M. Adams and A.I. Creagh 80 (1983) 379

Energy transfer and conversion

Exchange reactions of hydrogen halides with hydrogenic atoms, D.C. Clary 71 (1982) 117
Evaluation of an upper bound of the maximal Lyapunov characteristic number by Monte Carlo integration in the chaotic regions of phase space, S.C. Farantos 71 (1982) 157
X-ray scattering factors, Compton profiles, and shell corrections from numerical atomic wavefunctions, J. Oddershede and J.R. Sabin 71 (1982) 161
Intermolecular energy-transfer probabilities of strong colliders, O. Herscovitz, E. Tzidoni and I. Oref 71 (1982) 221
Fermi-coupled spherically adapted effective states in the collisionless multiphoton excitation of SF_6, C. di Lauro and F. Lattanzi 71 (1982) 233
Spectroscopic analysis of the vibrational distributions in dissociative CO–He RF discharges, S. de Benedictis, R. d'Agostino and F. Cramarossa 71 (1982) 247
A semiclassical model for the vibrational excitation of spherical-top molecules in collisions with ions, T. Ellenbroek and J.P. Toennies 71 (1982) 309
Photochemical control of energy transfer in molecular crystals, J.S. Patel and D.M. Hanson 72 (1982) 35
Evidence for the existence of structures in gas-phase homomolecular clusters of water, V. Hermann, B.D. Kay and A.W. Castleman Jr. 72 (1982) 185
Polarization of $CN(B\,^2\Sigma^+–X\,^2\Sigma^+)$ emission produced in the electron-impact dissociation of HCN and DCN, T. Nagata, T. Kondow and K. Kuchitsu 72 (1982) 281
Random coupling models. IV. Numerical investigation of the dependence on the random coupling distribution and on the initial phases, B. Carmeli, R. Tulman, A. Nitzan and M.H. Kalos 72 (1982) 363
The motion of triplet excitons in β-phase crystals of 9,10-dichloroanthracene, R. Krauss, W. Schrof, H.C. Wolf and D. Schmid 73 (1982) 55

Concurrence of the $n\nu_3$ and $(n-1)\nu_3+\nu_2+\nu_6$ vibrational ladders in the collisionless multiphoton excitation of $^{32}SF_6$, C. di Lauro, F. Lattanzi and G. Sanna 73 (1982) 215
The Franck–Condon principle for radiationless transitions in molecules and a selection rule for Morse oscillators, E.S. Medvedev 73 (1982) 243
Vibrational deactivation of CO(v = 1) by p-H_2 and o-H_2, L.L. Poulsen and G.D. Billing 73 (1982) 313
Classical differential cross sections and rotational energy transfer distributions for realistic ion–molecule potentials in the CPST limit, F.E. Budenholzer and C.-C. Lee 73 (1982) 323
Relaxation of the individual vibrational levels of carbon monoxide following shock heating at 2100 K, J.P. Martin, M.R. Buckingham, J.A. Chenery and C.J.S.M. Simpson 74 (1983) 15
Vibrational–translational/rotational and vibrational–vibrational processes in methane/inert-gas mixtures: optoacoustic phase measurements, E. Avramides and T.F. Hunter 74 (1983) 25
Vibrational relaxation times in polyatomic gas mixtures: on the validity of the linear mixture rule, Y.V. Chalapati Rao and B.V. Mallu 74 (1983) 43
Energy-transfer reactions between He($2\,^3S$) and Ne($^3P_{0,2}$) metastable atoms and PN radicals, H. Obase, M. Tsuji and Y. Nishimura 74 (1983) 89
Semiclassical theory for atom–surface scattering: calculations on Ar + W(110), G.D. Billing 74 (1983) 143
Detection of transient laser magnetic resonance signals in pulsed CO_2 laser irradiation of SF_6/H_2O and SF_6/NO mixtures, J.S. Geiger, D.R. Smith and J.D. Bonnett 74 (1983) 239
Photofragmentation of H_2S in the first continuum, G.N.A. van Veen, K.A. Mohamed, T. Baller and A.E. de Vries 74 (1983) 261
Quantum vibrational transition probabilities from real classical trajectories: asymmetric diatom–diatom collisions, R.T. Skodje, W.R. Gentry and C.F. Giese 74 (1983) 347
The unimolecular dissociation of electronic state-selected methyl iodide cations, I. Powis 74 (1983) 421
Classical trajectory study of three-body direct photofragmentation of $Cd(CH_3)_2$. Comparison of sampling methods, M.D. Pattengill 75 (1983) 59
Trajectory surface-hopping study of the K + O_2 collision: energy transfer in neutral and ionic products, G. Parlant, M. Schröder and S. Goursaud 75 (1983) 175
A model of localization, soliton propagation, and self-trapping in an electronically excited atomic lattice, M.A. Collins and D.P. Craig 75 (1983) 191
Reactions induced by ion bombardment of solid cyclohexane at 77 K, O. Puglisi, G. Marletta, S. Pignataro and G. Foti 75 (1983) 417
Chaotic motions in vibrating molecules: the generalized Hénon–Heiles model, R. Ramaswamy 76 (1983) 15
Luminescent charge transfer of ground-state and metastable B^+ ions, Ch. Ottinger, J. Reichmuth and M. Yang 76 (1983) 61
Vibrational energy disposal in reactions of fluorine atoms with hydrides of groups III, IV and V, A.S. Manocha, D.W. Setser and M.A. Wickramaaratchi 76 (1983) 129
Binary theory of dephasing in liquid solutions. I. The non-markovian theory of encounters, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 149
Binary theory of dephasing in liquid solutions. II. Motion-transformed isotropic Raman spectra, A.A. Kipriyanov, A.B. Doktorov and A.I. Burshtein 76 (1983) 163
Rate constants for vibrational energy transfer between CO(v = 1) and CH_4 and substituted methane molecules in the temperature range 300 to 80 K, D.C. Allen and C.J.S.M. Simpson 76 (1983) 231
Diatomics-in-molecules potential energy surfaces of $(HeH_2)^+$: an extended basis set calculation, F. Schneider, L. Zülicke, R. Polák and J. Vojtík 76 (1983) 259
Semiclassical calculation of energy transfer in polyatomic molecules. VIII. Theory for atom + non-linear triatom, G.D. Billing 76 (1983) 315
New type rotational basis function for quantum-mechanical molecular collision calculations, D.C. Clary 76 (1983) 331

The description of molecular large-amplitude motions in terms of curvilinear coordinates associated with the reaction path, A. Nauts and X. Chapuisat 76 (1983) 349
Infrared-induced conformational isomerization of ethylene glycol in a low-temperature argon matrix, H. Takeuchi and M. Tasumi 77 (1983) 21
Raman analysis of SF_6 molecular beams excited by a cw CO_2 laser, G. Luijks, J. Timmerman, S. Stolte and J. Reuss 77 (1983) 169
Delayed fluorescence ODMR and EPR studies of triplet excitons in charge-transfer molecular crystals, G. Agostini, C. Corvaja, G. Giacometti and L. Pasimeni 77 (1983) 233
Collinear collisions in a well potential, Ch.G. Schlier 77 (1983) 267
Monte Carlo calculations on unimolecular reactions, energy transfer, and IR-multiphoton decomposition, J.R. Barker 77 (1983) 301
Phosphorescence and E-type delayed fluorescence from azulene in phenazine host crystals, D. Klemp and B. Nickel 78 (1983) 17
He–HF vibrational inelasticity at low and intermediate energies from quantum collision theory, F.A. Gianturco, U.T. Lamanna and G. Petrella 78 (1983) 81
Surface hopping trajectory calculations for electronic rotational and vibrational inelastic collision for the Na–N_2 system, P. Archirel and P. Habitz 78 (1983) 213
Classical trajectory study of the effects of parent-molecule bending and overall rotation in polyatomic direct photofragmentation. Model ICN + $h\nu \rightarrow$ CN + I, M.D. Pattengill 78 (1983) 229
Dynamics of energy transport in ternary molecular solids. II. Time evolution of naphthalene fluorescence, P. Argyrakis and R. Kopelman 78 (1983) 251
Infrared laser photoisomerization of 2-fluoroethanol in argon, W.F. Hoffman III and J.S. Shirk 78 (1983) 331
Collisional and radiational energy transfer in the system $Na^*(3\,^2P) + Na_2(X\,^1\Sigma^+) \rightarrow Na(3\,^2S) + Na_2^*(A\,^1\Sigma^+)$, P. Arrowsmith, S.H.P. Bly, P.E. Charters, P. Chevrier, J.C. Polanyi and H.H. Telle 79 (1983) 31
Rotational and vibrational distributions of $N_2(C\,^3\Pi_u)$ excited by state-selected $Ar(^3P_2)$ and $Ar(^3P_0)$ metastable atoms, T.D. Nguyen and N. Sadeghi 79 (1983) 41
Dispersive singlet exciton motion in an organic glass, R. Jankowiak and H. Bässler 79 (1983) 57
A comparison of quantal and semiclassical perturbed-rotational-state methods in H^+–CO collisions, K. Sakimoto 79 (1983) 137
Theoretical investigation of rotational rainbows in K + N_2 and K + CO collisions, D. Häusler and R. Schinke 79 (1983) 147
Breathing-sphere quantum calculations of integral and differential cross sections for vibrational excitation in ion (atom)–diatom collisions, G. Drolshagen and J.P. Toennies 79 (1983) 159
Semiclassical calculation of energy transfer in polyatomic molecules. X. Energy transfer in Ar + SF_6 at 1 eV, G.D. Billing 79 (1983) 179
Fluorescence lifetime and collisional quenching of the predissociative NO $B\,^2\Pi(v' = 7)$ state, K. Shibuya and F. Stuhl 79 (1983) 367
Formation of $NH(A\,^3\Pi, C\,^1\Pi)$ by electron-impact dissociation of HN_3, I. Tokue and Y. Ito 79 (1983) 383
Vibrational energy relaxation of highly compressed gaseous H_2 and N_2, M. Châtelet, J. Kieffer and B. Oksengorn 79 (1983) 413
The theory of transitions between electronic states. Application to radiationless transitions in polar solvents, L.D. Zusman 80 (1983) 29
New I_2 emission from iodine atom recombination reaction, K.-H. Stephan-Rossbach and F.J. Comes 80 (1983) 121
Vibrational effects with excitation transfer in metastable rare-gas–halide collisions, M.S. de Vries and R.M. Martin 80 (1983) 157
Radiative lifetime and quenching of $SO(b\,^1\Sigma^+, v' = 0)$, J. Wildt, E.H. Fink, R. Winter and F. Zabel 80 (1983) 167

Theory of coherence effects in time dependent delayed fluorescence. II. Application to two- and three-dimensional crystals, A. Fort, V. Ern and V.M. Kenkre 80 (1983) 205
Semiclassical calculation of energy transfer in polyatomic molecules. IX. Cross sections for $M + CO_2(000) \rightarrow M + CO_2(nml)$ (M = He and Ar), G.D. Billing and D.C. Clary 80 (1983) 213
Singlet exciton migration in a random organic two-component system containing physical and chemical traps, G. Peter, B. Ries and H. Bässler 80 (1983) 289
Intensity dependence of CO_2-laser-induced multiphoton absorption and decomposition of monomethylamine, D.K. Evans, R.D. McAlpine, H.M. Adams and A.L. Creagh 80 (1983) 379

Reactions
Are atoms intrinsic to molecular electronic wavefunctions? I. The FORS model, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 41
Are atoms intrinsic to molecular electronic wavefunctions? II. Analysis of FORS orbitals, K. Ruedenberg, M.W. Schmidt and M.M. Gilbert 71 (1982) 51
Are atoms intrinsic to molecular electronic wavefunctions? III. Analysis of FORS configurations, K. Ruedenberg, M.W. Schmidt, M.M. Gilbert and S.T. Elbert 71 (1982) 65
Exchange reactions of hydrogen halides with hydrogenic atoms, D.C. Clary 71 (1982) 117
Analysis of the steric dependence of the CH_3I + Rb reaction using a Legendre expansion technique, S. Stolte, K.K. Chakravorty, R.B. Bernstein and D.H. Parker 71 (1982) 353
Polymerization of TS-12 diacetylene crystals: crystal structures of monomer and polymer and spectroscopy of reaction intermediates, D. Siegel, H. Sixl, V. Enkelmann and G. Wenz 72 (1982) 201
Polarization of $CN(B\,^2\Sigma^+ - X\,^2\Sigma^+)$ emission produced in the electron-impact dissociation of HCN and DCN, T. Nagata, T. Kondow and K. Kuchitsu 72 (1982) 281
Calculations on the mechanism of ion polymerization in the formaldehyde crystal, M.V. Basilevsky, G.N. Gerasimov and S.I. Petrochenko 72 (1982) 349
On the connection between incubation and relaxation times in thermal unimolecular reactions, H.O. Pritchard and S.R. Vatsya 72 (1982) 447
Temperature dependence of the reaction of CH radicals with unsaturated hydrocarbons, M.R. Berman, J.W. Fleming, A.B. Harvey and M.C. Lin 73 (1982) 27
Positronium yields in liquids determined by lifetime and angular correlation measurements, O.E. Mogensen and F.M. Jacobsen 73 (1982) 223
Photodissociation of molecular beams of SO_2 at 193 nm, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 73 (1982) 377
Photochemical decay of butynal ($H_3CC{\equiv}C{-}CHO$) in the gas phase following $S_1(n\pi^*) \leftarrow S_0$ excitation, H.U. Zürcher, U. Brühlmann and J.R. Huber 73 (1982) 403
Temperature dependence of $C_3(X\,^1\Sigma_g^+)$ reactions with alkenes and alkynes, 295–610 K, H.H. Nelson, H. Helvajian, L. Pasternack and J.R. McDonald 73 (1982) 431
Quantum-mechanical rearrangement processes: off-shell vibrorotational sudden approximation to the dynamics, E. Ficocelli Varracchio 74 (1983) 153
A theoretical study of the condensation reactions of methyl cation with ammonia, water, hydrogen fluoride and hydrogen sulphide, R.H. Nobes and L. Radom 74 (1983) 163
Detection and identification of free radicals in the gaseous-phase ozonolysis of ethylene: microreactor–matrix ESR spectroscopy, F.J. Rákóczi, T.-K. Ha and Hs.H. Günthard 74 (1983) 273
An efficient solutions of weak-collision master equations in thermal unimolecular reaction rate theory, H.W. Schranz and S. Nordholm 74 (1983) 365
The unimolecular dissociation of electronic state-selected methyl iodide cations, I. Powis 74 (1983) 421
Kinetics of methyl radical reaction with methanol at 20–105 K, V.L. Vyazovkin, B.V. Bol'shakov and V.A. Tolkatchev 75 (1983) 11

Benchmark measurement of iodobenzene ion fragmentation rates, J. Dannacher, H.M. Rosenstock, R. Buff, A.C. Parr, R.L. Stockbauer, R. Bombach and J.-P. Stadelmann 75 (1983) 23
The orientation-averaged rotation-decoupled vibration model for product state distributions in light+heavy–heavy reactions, W. Jakubetz 75 (1983) 45
Semi-emperical corrections to the mixing coefficients for the diatomics-in-molecules method, P.J. Kuntz and C.C. Chang 75 (1983) 79
Two-frequency CO_2 laser multiple-photon dissociation and dynamics of excited state absorption in CDF_3, I.P. Herman 75 (1983) 121
Vibrationally excited molecules and mechanisms of chemical and physical processes in non-equilibrium plasmas, P.A. Sergeev and D.I. Slovetsky 75 (1983) 231
Reactions induced by ion bombardment of solid cyclohexane at 77 K, O. Puglisi, G. Marletta, S. Pignataro and G. Foti 75 (1983) 417
Luminescent charge transfer of ground-state and metastable B^+ ions, Ch. Ottinger, J. Reichmuth and M. Yang 76 (1983) 61
Vibrational energy disposal in reactions of fluorine atoms with hydrides of groups III, IV and V, A.S. Manocha, D.W. Setser and M.A. Wickramaaratchi 76 (1983) 129
Local normal modes and vibrational adiabatic potentials, N. Agmon 76 (1983) 203
Diatomics-in-molecules potential energy surfaces of $(HeH_2)^+$: an extended basis set calculation, F. Schneider, L. Zülicke, R. Polák and J. Vojtík 76 (1983) 259
New type of rotational basis function for quantum-mechanical molecular collision calculations, D.C. Clary 76 (1983) 331
The description of molecular large-amplitude motions in terms of curvilinear coordinates associated with the reaction path, A. Nauts and X. Chapuisat 76 (1983) 349
The dissociation energies of gaseous SmLi, EuLi, TmLi and YbLi, A. Neubert and K.F. Zmbov 76 (1983) 469
Some problems of recombination kinetics. I, E. Kotomin and V. Kuzovkov 76 (1983) 479
Dynamics of formation of $CN(B\,^2\Sigma^+)$ fragment from HCN and DCN in an argon afterglow, Y. Ozaki, T. Kondow and K. Kuchitsu 77 (1983) 223
Dependence of photochemical and photophysical hole burning on laser intensity, A.U. Jalmukhambetov and I.S. Osad'ko 77 (1983) 247
Collinear collisions in a well potential, Ch.G. Schlier 77 (1983) 267
Ab initio study of the thermodynamic and kinetic stability of the ammonium radical, H. Cardy, D. Liotard, A. Dargelos and E. Poquet 77 (1983) 287
Monte Carlo calculations on unimolecular reactions, energy transfer, and IR-multiphoton decomposition, J.R. Barker 77 (1983) 301
An NMR relaxation study of hydrogen exchange and its deuterium isotope effects in aqueous carboxylic acid solutions, D. Lankhorst, J. Schriever and J.C. Leyte 77 (1983) 319
The nascent translational energy of difluorocarbene produced in IR MPD of the penta-fluoroethyl radical, D.M. Rayner, S. Kimel and P.A. Hackett 77 (1983) 349
Spectroscopic studies of the photochromism of N-salicylideneaniline mixed crystals and glasses, D. Higelin and H. Sixl 77 (1983) 391
The kinetics of the retarded reaction of free radicals with oxygen in a methanol glass, V.A. Bagryansky, V.M. Zaskul'nikov and V.A. Tolkatchev 78 (1983) 41
Photolytic production of $O(^3P)$ in the presence of CF_3I: the formation of $IF(X\,^1\Sigma^+)$, T.A. Watson, M. Addison and C. Wittig 78 (1983) 57
Photodissociation of molecular beams of N_2O_4, M. Kawasaki, K. Kasatani, H. Sato, H. Shinohara and N. Nishi 78 (1983) 65
Theoretical three-dimensional potential-energy surface for the reaction of Be with HF, S. Chapman, M. Dupuis and S. Green 78 (1983) 93

Classical trajectory study of the effects of parent-molecule bending and overall rotation in polyatomic direct photofragmentation. Model ICN + $h\nu \rightarrow$ CN + I, M.D. Pattengill 78 (1983) 229
Separation of deuterium IR multiphoton decomposition of chlorodifluoromethane. IR multiphoton absorption by and decomposition of a CF_2DCl/CF_2HCl mixture, K.O. Kutschke, M. Gauthier and P.A. Hackett 78 (1983) 323
Infrared laser photoisomerization of 2-fluoroethanol in argon, W.F. Hoffman III and J.S. Shirk 78 (1983) 331
State-selected molecular-beam reaction dynamics of K with HF (v = 1, j = 5,6 and 7), M. Hoffmeister, L. Potthast and H.J. Loesch 78 (1983) 369
Bifurcation diagrams for two substrate oscillatory systems, J. Maselko 78 (1983) 381
Kinetic studies of the bromine–oxygen system: a new paramagnetic particle, BrO_2, N.I. Butkovskaya, I.I. Morozov, V.L. Tal'rose and E.S. Vasiliev 79 (1983) 21
Flash photolysis electron spin resonance and CIDEP studies of radicals derived from nitrogen heterocyclics. I. The diazanaphthalenes, S. Basu, K.A. McLauchlan and A.J.D. Ritchie 79 (1983) 95
Prediction and interpretation of collinear reactive scattering resonances by the diagonal corrected vibrational adiabatic hyperspherical model, J. Römelt 79 (1983) 197
On the theory of adiabatic electron-transfer reactions in polar solvents, A.B. Helman 79 (1983) 235
Deuterium separation and infrared photochemistry in CF_2HCl, J. Moser, P. Morand, R. Duperrex and H. van den Bergh 79 (1983) 277
Search for the laser-induced crossed beam reaction of excited $I_2(B\,^3\Pi)$ with Hg, M.M. Oprysko, F.J. Aoiz, R.B. Bernstein and M.A. McMahan 79 (1983) 341
Kinetics and detection of F(^{2}P) atoms in a discharge flow system, M.A.A. Clyne and A. Hodgson 79 (1983) 351
Charge transfer in polar media. Transition-state entropy, Yu.I. Dakhnovskii and A.A. Ovchinnikov 80 (1983) 17
The theory of transitions between electronic states. Application to radiationless transitions in polar solvents, L.D. Zusman 80 (1983) 29
New I_2 emission from iodine atom recombination reaction, K.-H. Stephan-Rossbach and F.J. Comes 80 (1983) 121
Determination of rate constants for some reactions of CBr radicals by VUV laser flash photolysis, L. Hellner, K.T.V. Grattan and M.H.R. Hutchinson 80 (1983) 345

Intermolecular interactions

The direct reaction field hamiltonian: analysis of the dispersion term and application to the water dimer, B.T. Thole and P.Th. van Duijnen 71 (1982) 211
Intermolecular energy-transfer probabilities of strong colliders, O. Herscovitz, E. Tzidoni and I. Oref 71 (1982) 221
A semiclassical model for the vibrational excitation of spherical-top molecules in collisions with ions, T. Ellenbroek and J.P. Toennies 71 (1982) 309
State-to-state total cross sections for ion-pair formation, U.C. Klomp and J. Los 71 (1982) 443
Molecular dynamics computer simulation of liquid dichloromethane. I. Equilibrium properties, M. Ferrario and M.W. Evans 72 (1982) 141
Compute simulation of dichloromethane. II. Molecular dynamics, M. Ferrario and M.W. Evans 72 (1982) 147
Ab initio calculation of the equilibrium geometry and the ^{13}C, ^{17}O and ^{27}Al NMR chemical shielding tensors of the system Al^{3+}/CO, Th. Weller, W. Meiler, A. Michael, H.J. Köhler, H. Lischka and R. Höller 72 (1982) 155
Phonon spectra and structure of crystalline ethylene oxide and ethylene sulphide at 77 K, R. Cataliotti and G. Paliani 72 (1982) 293

Collision-induced absorption in a He–Ar mixture, A. Raczyński 72 (1982) 321
Laser-induced ultrasonics: a dynamic holographic approach to the measurement of weak absorptions, optoelastic constants and acoustic attenuation, R.J.D. Miller, R. Casalegno, K.A. Nelson and M.D. Fayer 72 (1982) 371
Glory undulations in the total cross section for Ar–Ar, Kr, Xe and Kr–Ar, Kr, H.C.W. Beijerinck, P.M.A. van der Kam and N.F. Verster 72 (1982) 391
A study of picosecond dehalogenation of chlorobenzene anions in liquids by positronium inhibition measurements, G. Wikander and O.E. Mogensen 72 (1982) 407
On the structure and dynamics of liquid benzene, O. Steinhauser 73 (1982) 155
Some observations on molecular complexes of carbon monoxide in argon and oxygen matrices, M. Diem, T.-L. Tso and E.K.C. Lee 73 (1982) 283
α- and β-phases of oxalic acid, $H_2C_2O_4$: vibrational spectra, normal-coordinate calculations, and intermolecular forces, J. de Villepin, A. Novak and D. Bougeard 73 (1982) 291
Classical differential cross sections and rotational energy transfer distributions for realistic ion–molecule potentials in the CPST limit, F.E. Budenholzer and C.-C. Lee 73 (1982) 323
Chiral discrimination in the liquid state: a hard-core model for the rôle of repulsive forces, D.P. Craig and I.R. Elsum 73 (1982) 349
Van der Waals forces and molecular diffraction from metal surfaces, with application to Ag(111), N.R. Hill, M. Haller and V. Celli 73 (1982) 363
The dual phosphorescence of benzophenazine in ethanol, G.W. Suter and U.P. Wild 73 (1982) 421
Vibrational relaxation of hydrogen-bonded species in solution. IV. Temperature and concentration dependence of the ν_σ(OH---N) band of phenol–pyridine, U.P. Agarwal, R.S. Green and I. Yarwood 74 (1983) 35
The rotational spectrum and molecular properties of a hydrogen-bonded dimer of phosphine and hydrogen fluoride, A.C. Legon and L.C. Willoughby 74 (1983) 127
Molecular interactions and reorientational motion of neat acetone in the liquid state. ^{17}O NMR chemical shifts and linewidths at variable temperature, B. Ancian, B. Tiffon and J.-E. Dubois 74 (1983) 171
Anharmonic processes in molecular crystals. Calculation of the anharmonic shifts, bandwidths and energy decay processes in crystalline naphthalene, R.D. Della Valle, P.F. Fracassi, R. Righini and S. Califano 74 (1983) 179
Electrostatic energy of vacancy formation in crystals of polar molecules, R.W. Munn 74 (1983) 301
Quantum vibrational transition probabilities from real classical trajectories: asymmetric diatom–diatom collisions, R.T. Skodje, W.R. Gentry and C.F. Giese 74 (1983) 347
Theoretical solvent effects on molecular structure and spectroscopic properties through the virtual-charge model. Application to the inverted solvatochromy of benzophenone $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ absorption bands, A. Botrel, F. Corre and A. le Beuze 74 (1983) 383
Vibrational relaxation of $CO_2(00^01)$ and $N_2O(00^01)$ by NO, F. Al Adel, L. Doyennette, M. Margottin-Maclou and L. Henry 74 (1983) 413
Classical trajectory study of three-body direct photofragmentation of $Cd(CH_3)_2$. Comparison of sampling methods, M.D. Pattengill 75 (1983) 59
Experimental and theoretical study of the vibrational relaxation of $CO(v = 1)$ and $N_2(v = 1)$: V–T relaxation by the isotopes of helium, M.M. Maricq, E.A. Gregory, C.T. Wickham-Jones, D.J. Cartwright and C.J.S.M. Simpson 75 (1983) 347
Fractionally charged ions in crystal lattices of organic ion-radical salts, L. Komorowski 76 (1983) 31
Fluorescence quenching of tertiary amines by halocarbons, P.C. Alford, C.G. Cureton, R.A. Lampert and D. Phillips 76 (1983) 103

Study of the dependence of spin–orbit matrix elements on AO basis set composition for inner and valence shells: results for the multiplet splitting of $X\,^3\Sigma^-$ and $C\,^3\Pi$ of SO and $X\,^2\Pi$ in SO^+, R. Klotz, C.M. Marian, S.D. Peyerimhoff, B.A. Hess and R.J. Buenker 76 (1983) 367
The temperature dependence of the structure of water, P.A. Egelstaff and J.H. Root 76 (1983) 405
Solvent effects on the potential energy surfaces of molecular iodine: a spectroscopic study, M. Geilhaupt and Th. Dorfmüller 76 (1983) 443
Dynamics of a prototype alkali–hydrogen-halide exchange reaction on an ab initio potential-energy surface, I. Noorbatcha and N. Sathyamurthy 77 (1983) 67
Inhibition of Ps formation in benzene and cyclohexane by CH_3Cl and CH_3Br. Correlation to radiation chemistry results, G. Wikander, O.E. Mogensen and N.-J. Pedersen 77 (1983) 159
Hopping transport and energy transfer in substitutionally disordered media, B. Sipp 77 (1983) 257
Generalized Landau–Zener formula for non-adiabatic transitions between degenerate states, V.V. Likhansky and G.A. Solodovnikov 77 (1983) 409
Long-range interactions of Li(n = 2) states with each other and the long-range interaction of Li($2s\,^2S$) with Li($3s\,^2S$), D.D. Konewalow and J.L. Fish 77 (1983) 435
The mechanism of fluorescence quenching of aromatic compounds by acids: ZDO calculations, S.I. Druzhinin and B.M. Uzhinov 78 (1983) 29
Theoretical three-dimensional potential-energy surface for the reaction of Be with HF, S. Chapman, M. Dupuis and S. Green 78 (1983) 93
Interaction potentials for Li^+–rare-gas systems, L.A. Viehland 78 (1983) 279
On the Ne–Ne potential energy curve and related properties, R.A. Aziz, W.J. Meath and A.R. Allnatt 78 (1983) 295
The effect of molecular excitation on crystal packing. 9-cyano- and 9,10-dimethyl-anthracene as excited guest/host and host/guest pairs, K. Norris, P. Gray, D.P. Craig, C.P. Mallett and B.R. Markey 79 (1983) 9
Rotational and vibrational distributions of $N_2(C\,^3\Pi_u)$ excited by state-selected $Ar(^3P_2)$ and $Ar(^3P_0)$ metastable atoms, T.D. Nguyen and N. Sadeghi 79 (1983) 41
A quantitative analysis of the ν_s (IR) bands of H-bonds. I. Theory, Y. Marechal 79 (1983) 69
A quantitative analysis of the ν_s (IR) bands of H-bonds. II. Adipic acid crystals, Y. Marechal 79 (1983) 85
Theoretical investigation of rotational rainbows in K + N_2 and K + CO collisions, D. Häusler and R. Schinke 79 (1983) 147
Breathing-sphere quantum calculations of integral and differential cross sections for vibrational excitation in ion (atom)–diatom collisions, G. Drolshagen and J.P. Toennies 79 (1983) 159
Ab initio studies on hydrogen-bonded chains. III. The linear, infinite chain of hydrogen cyanide molecules, A. Karpfen 79 (1983) 211
Theory of sorption of gases on polymers. II. Effects of inter-chain secondary bonds, M. Pyda and M. Kurzyński 79 (1983) 219
Quasi-elastic light scattering studies on T7 DNA in the presence of a sinusoidal electric field, K.S. Schmitz 79 (1983) 297
Secondary amines: a low-temperature dielectric relaxation study, J. Gilchrist and H. Godfrin 79 (1983) 307
Vibrational energy relaxation of highly compressed gaseous H_2 and N_2, M. Châtelet, J. Kieffer and B. Oksengorn 79 (1983) 413
On the dielectric theory and computer simulation of water, O. Steinhauser 79 (1983) 465
Electronic spectroscopy of fluorobenzene van der Waals molecules by resonant two-photon ionization, K. Rademann, B. Brutschy and H. Baumgärtel 80 (1983) 129
Conformational energetics in hydrogen-bonded dimers. The unobserved CO–HF complex, M.A. Benzel and C.E. Dykstra 80 (1983) 273

Ionic and excited state phenomena
Features of the photochemically active state surface of azobenzene, S. Monti, G. Orlandi and P. Palmieri 71 (1982) 87
Emission and laser excitation spectra of rotationally cooled cations in the gas phase: $\tilde{A}\,^2\Pi \leftrightarrow \tilde{X}\,^2\Pi$ band systems of $H(C{\equiv}C)_2X^+$, X = Cl, Br, D. Klapstein, J.P. Maier, L. Misev and W. Zambach 72 (1982) 101
Potential energy curves and transition moments for the two-lying electronic states of the Si_2 molecule, S.D. Peyerimhoff and R.J. Buenker 72 (1982) 111
Unimolecular dissociations of excited $C_3H_6O^+$: a comparative photoelectron–photoion coincidence study of 1,2-epoxypropane and acetone, R. Bombach, J.-P. Stadelmann and J. Vogt 72 (1982) 259
A study of picosecond dehalogenation of chlorobenzene anions in liquids by positronium inhibition measurements, G. Wikander and O.E. Mogensen 72 (1982) 407
Photon-induced molecular charge separation studied by nanosecond time-resolved microwave conductivity, M.P. de Haas and J.M. Warman 73 (1982) 35
Autoionization in HCl and DCl by photoelectron spectroscopy, P. Natalis, P. Pennetreau, L. Longton and J.E. Collin 73 (1982) 191
Raman spectroscopy from a picosecond-lived excited state of methyl orange, L.V. Haley and J.A. Koningstein 73 (1982) 263
Dissociation cross sections of silane and disilane by electron impact, J. Perrin, J.P.M. Schmitt, G. de Rosny, B. Drevillon, J. Huc and A. Lloret 73 (1982) 383
Absolute dipole oscillator strengths for molrcular and dissociative photoionization of hydrogen fluoride, F. Carnovale and C.E. Brion 74 (1983) 253
The unimolecular dissociation of electronic state-selected methyl iodide cations, I. Powis 74 (1983) 421
Unusual low-energy isomers for simple radical cations, M.J. Frisch, K. Raghavachari, J.A. Pople, W.J. Bouma and L. Radom 75 (1983) 323
Internal energy dependence of the autodetachment and dissociation of the SF_6^- ion, J.P. Astruc, R. Barbé, A. Lagrèze and J.P. Schermann 75 (1983) 405
Cluster expansion of the wavefunction. Valence and Rydberg excitations, ionizations, and inner-valence ionizations of CO_2 and N_2O studied by the SAC CI theories, H. Nakatsuji 75 (1983) 425
Luminescent charge transfer of ground-state and metastable B^+ ions, Ch. Ottinger, J. Reichmuth and M. Yang 76 (1983) 61
Kinetic energy release distribution in the fragmentation of energy-selected iodopropane ions, W.A. Brand, T. Baer and C.E. Klots 76 (1983) 111
Unified theory of the electronic Stark effect in molecular crystals, R.W. Munn 76 (1983) 243
Cluster expansion of the wavefunction. Outer- and inner-valence ionization spectra of CS_2 and COS, H. Nakatsuji 76 (1983) 283
The N1s shake-up spectrum of para-aminobenzonitrile. A theoretical and experimental ESCA study, P.-Å. Malmquist, S. Svensson and H. Ågren 76 (1983) 429
Long-range interactions of Li(n = 2) states with each other and the long-range interaction of Li($2s\,^2S$) with Li($3s\,^2S$), D.D. Konowalow and J.L. Fish 77 (1983) 435
Emission spectra of rotationally cooled dihaloacetylene cations in the gas phase: $\tilde{A}\,^2\Pi_{\Omega,g} \rightarrow \tilde{X}\,^2\Pi_{\Omega,u}$ band systems, D. Klapstein, J.P. Maier and W. Zambach 77 (1983) 463
Accessibility of the lowest quintet state of organic molecules through triplet–triplet annihilation; an INDO CI study, B. Dick and B. Nickel 78 (1983) 1
Phosphorescence and E-type delayed fluorescence from azulene in phenazine host crystals, D. Klemp and B. Nickel 78 (1983) 17

The mechanism of fluorescence quenching of aromatic compounds by acids: ZDO calculations, S.I. Druzhinin and B.M. Uzhinov 78 (1983) 29
Emission spectra of supersonically cooled methyldiacetylene cations, S. Leutwyler, D. Klapstein and J.P. Maier 78 (1983) 151
Emission spectra of supersonically cooled dimethyldiacetylene cations, D. Klapstein, R. Kuhn, S. Leutwyler and J.P. Maier 78 (1983) 167
Complete valence-shell ionization spectra of N_2 and CO: application of the extended two-particle–hole Tamm–Dancoff approximation (2ph-TDA), J. Schirmer and O. Walter 78 (1983) 201
Semiclassical theory of predissociation induced by rotational (Coriolis) coupling, H. Nakamura 78 (1983) 235
High-resolution UV photoelectron spectrum of CO_2, I. Reineck, C. Nohre, R. Maripuu, P. Lodin, S.H. Al-Shamma, H. Veenhuizen, L. Karlsson and K. Siegbahn 78 (1983) 311
Valence-shell photoabsorption by CO_2 and its connections with electron–CO_2 scattering, P.M. Dittman, D. Dill and J.L. Dehmer 78 (1983) 405
Rotational and vibrational distributions of $N_2(C\,^3\Pi_u)$ excited by state-selected $Ar(^3P_2)$ and $Ar(^3P_0)$ metastable atoms, T.D. Nguyen and N. Sadeghi 79 (1983) 41
Can the H_5 molecule be observed?, K. Kaufmann, M. Jungen and V. Staemmler 79 (1983) 111
Argon ion laser excitation of supersonic seeded molecular beams of I_2, F.J. Aoiz, M.M. Oprysko and R.B. Bernstein 79 (1983) 321
Breakdown in the Koopmans' theorem interpretation of the outer valence-level photoemission spectra of selected organic molecules, R.W. Bigelow 80 (1983) 45
Radiative lifetime and quenching of $SO(b\,^1\Sigma^+, v' = 0)$, J. Wildt, E.H. Fink, R. Winter and F. Zabel 80 (1983) 167
The effect of a magnetic field on discrete and continuum CS_2 fluorescence, S.J. Silvers, M.R. McKeever and G.K. Chawla 80 (1983) 177
Comparison of photon-stimulated dissociation of gas-phase, solid and chemisorbed water, D.E. Ramaker 80 (1983) 183
Dissociative excitation of SiH_4, SiD_4, Si_2H_6 and GeH_4 by 0–100 eV electron impact, J. Perrin and J.F.M. Aarts 80 (1983) 351
Infrared-enhanced multiphoton dissociation of iodobenzene cations, N.B. Lev and R.C. Dunbar 80 (1983) 367

Ionization

Electronic properties by Green's function calculations. Renormalized optical potential results: Ne, Ar, HF, H_2O, NH_3, I. Cacelli, R. Moccia and V. Carravetta 71 (1982) 199
Atoms-in-molecules calculations on diatomic fragments of polyatomic systems: HeH, HeH^+ and HeH^- for a DIM model of Penning ionization of H_2 by He*, I. Paidarová, J. Vojtík and R. Polák 72 (1982) 119
Photoelectron spectra and their relativistic interpretation for gaseous bismuth trihalides, R.G. Egdell, M. Hotokka, L. Laaksonen, P. Pyykkö and J.G. Snijders 72 (1982) 237
Unimolecular dissociations of excited $C_3H_6O^+$: a comparative photoelectron–photoion coincidence study of 1,2-epoxypropane and acetone, R. Bombach, J.-P. Stadelmann and J. Vogt 72 (1982) 259
Intense shake-up satellites in the XPS spectra of planar and sterically hindered N-piperidyl-nitrobenzenes and -nitrothiophens, G. Distefano, M. Guerra, F.P. Colonna, D. Jones, G. Consiglio and D. Spinelli 72 (1982) 267
Dissociation cross sections of silane and disilane by electron impact, J. Perrin, J.P.M. Schmitt, G. de Rosny, B. Drevillon, J. Huc and A. Lloret 73 (1982) 383

Photoelectron spectroscopic study of simple hydrogen-bonded dimers. I. Supersonic nozzle beam photoelectron spectrometer and the formic-acid dimer, S. Tomoda, Y. Achiba, K. Nomoto, K. Sato and K. Kimura 74 (1983) 113
Photoelectron spectroscopic study of simple hydrogen-bonded dimers. II. The methanol dimer, S. Tomoda and K. Kimura 74 (1983) 121
A theoretical study of the condensation reactions of methyl cation with ammonia, water, hydrogen fluoride and hydrogen sulphide, R.H. Nobes and L. Radom 74 (1983) 163
Angle-resolved photoelectron measurements on the 2p orbitals of Si in SiF_4 and $Si(CH_3)_4$ in the gas phase, P.R. Keller, J.W. Taylor, F.A. Grimm, P. Senn, T.A. Carlson and M.O. Krause 74 (1983) 247
Trajectory surface-hopping study of the $K + O_2$ collision: energy transfer in neutral and ionic products, G. Parlant, M. Schröder and S. Goursaud 75 (1983) 175
Unusual low-energy isomers for simple radical cations, M.J. Frisch, K. Raghavachari, J.A. Pople, W.J. Bouma and L. Radom 75 (1983) 323
A combination of pseudopotentials and density functionals: results for Li_n^{m+}, Na_n^{m+} and K_n^{m+} clusters ($n \leqslant 4; m = 0,1$), J. Flad, G. Igel, M. Dolg, H. Stoll and H. Preuss 75 (1983) 331
Ionization potentials and polarization energies of tetraselenafulvalene (TSF) derivatives determined from ultraviolet photoelectron spectroscopy, N. Sato, G. Saito and H. Inokuchi 76 (1983) 79
Molecular orbital electron momentum distribution and separation energies of CH_3CN, A. Minchinton, C.E. Brion, J.P.D. Cook and E. Weigold 76 (1983) 89
Kinetic energy release distribution in the fragmentation of energy-selected iodopropane ions, W.A. Brand, T. Baer and C.E. Klots 76 (1983) 111
MS Xα and LCAO Xα calculations of ionization potentials. A comparison with Koopmans' theorem and accurate calculations, G. de Alti, P. Decleva and A. Lisini 76 (1983) 185
Cluster expansion of the wavefunction. Outer- and inner-valence ionization spectra of CS_2 and COS, H. Nakatsuji 76 (1983) 283
Theoretical analysis of photoelectron angular distributions of linear molecules, W. Thiel 77 (1983) 103
Two-photon ionization and dissociation of liquid water by powerful laser UV radiation, D.N. Nikogosyan, A.A. Oraevsky and V.I. Rupasov 77 (1983) 131
Charge transfer to a solvent state. VIII. Localization of charge during the transition state of the solute: the solute cation localization energy, T.B. Truong 77 (1983) 377
Generalized Landau–Zener formula for non-adiabatic transitions between degenerate states, V.V. Likhansky and G.A. Solodovnikov 77 (1983) 409
Proper characterization of MC SCF stationary points, J.T. Golab, D.L. Yeager and P. Jørgensen 78 (1983) 175
Complete valence-shell ionization spectra of N_2 and CO: application of the extended two-particle–hole Tamm–Dancoff approximation (2ph-TDA), J. Schirmer and O. Walter 78 (1983) 201
EOM/propagator ionization potentials: extension of the excitation operator manifold, J. Baker 79 (1983) 117
Angle-resolved photoelectron spectroscopy of the chloro-substituted methanes, P.R. Keller, J.W. Taylor, T.A. Carlson and F.A. Grimm 79 (1983) 269
Theoretical study of shake-up in the core photoelectron spectra of the alkali atoms, G. de Alti, P. Decleva and A. Lisini 80 (1983) 229
Autoionization spectra of Li_2 and the $X\,^2\Sigma_g^+$ ground state of Li_2^+: experimental and theoretical investigations, D. Eisel, W. Demtröder, W. Müller and P. Botschwina 80 (1983) 329
Angular distribution for the major photoelectron bands of nitrogen below 45 eV binding energy, F.A. Grimm and Th.A. Carlson 80 (1983) 389

Isotope effects
Multiphoton dissociation of some volatile uranyl complexes. I. The phenomena of reversible and permanent dissociation, J.E. Eberhardt, I.E. Hoare, D.A. Johnson, R.B. Knott, A.W. Pryor and A.B. Waugh 72 (1982) 41
Multiphoton dissociation of some volatile uranyl complexes. II. Frequency and isotopic effects, J.E. Eberhardt, R.B. Knott and A.W. Pryor 72 (1982) 51
Electronic–vibrational excitations of a hydrogen-bonded molecule in supersonic expansions: 1,4-dihydroxyanthraquinone and its deuterated derivatives, G. Smulevich, A. Amirav, U. Even and J. Jortner 73 (1982) 1
Electron impact dissociation of molecular hydrogen and deuterium: isotope effect on the emission cross section of H^* and D^* (n = 3, 4, 5), M. Higo, S. Kamata and T. Ogawa 73 (1982) 99
Muonium-substituted organic free radicals in liquids. Muon–electron hyperfine coupling constants and the selectivity of formation of methyl- and fluorine-substituted cyclohexadienyl-type radicals, E. Roduner, G.A. Brinkman and P.W.F. Louwrier 73 (1982) 117
Autoionization in HCl and DCl by photoelectron spectroscopy, P. Natalis, P. Pennetreau, L. Longton and J.E. Collin 73 (1982) 191
Electron hopping and magnetic field dependent spin dynamics of radical ions in solution, H.W. Krüger, M.E. Michel-Beyerle and E.W. Knapp 74 (1983) 205
Detection and identification of free radicals in the gaseous-phase ozonolysis of ethylene: microreactor–matrix ESR spectroscopy, F.J. Rákóczi, T.-K. Ha and Hs.H. Günthard 74 (1983) 273
The dipole moment of ^{7}LiH and ^{7}LiD in the excited $A\,^1\Sigma^+$ state: a test of the Born–Oppenheimer approximation, M. Brieger, A. Renn, A. Sodeik and A. Hese 75 (1983) 1
Two-frequency CO_2 laser multiple-photon dissociation and dynamics of excited state absorption in CDF_3, I.P. Herman 75 (1983) 121
Measurement of the ^{14}N nuclear quadrupole couplings in the lowest ($n\pi^*$) excited triplet state of pyrazine by ODMR, W. Fröhling, C.J. Winscom and K. Möbius 75 (1983) 389
Photodissociation kinematics. II. Laboratory angular distributions of a hydride model system and the kinematic isotope effect, K.-M. Chen and C.-C. Pei 76 (1983) 219
Dynamics of formation of $CN(B\,^2\Sigma^+)$ fragment from HCN and DCN in an argon afterglow, Y. Ozaki, T. Kondow and K. Kuchitsu 77 (1983) 223
An NMR relaxation study of hydrogen exchange and its deuterium isotope effects in aqueous carboxylic acid solutions, D. Lankhorst, J. Schriever and J.C. Leyte 77 (1983) 319
Dielectric relaxation in cyano complexes of the $K_4Me^{II}(CN)_6 \cdot 3H_2O$ type. II. Isotopic effect, H.A. Kołodziej and S. Sorriso 78 (1983) 75
Separation of deuterium by IR multiphoton decomposition of chlorodifluoromethane. IR multiphoton absorption by and decomposition of a CF_2DCl/CF_2HCl mixture, K.O. Kutschke, M. Gauthier and P.A. Hackett 78 (1983) 323
Deuterium separation and infrared photochemistry in CF_2HCl, J. Moser, P. Morand, R. Duperrex and H. van den Bergh 79 (1983) 277
Dissociative excitation of SiH_4, SiD_4, Si_2H_6 and GeH_4 by 0–100 eV electron impact, J. Perrin and J.F.M. Aarts 80 (1983) 351

Surface effects
Synchrotron-radiation photoemission study of the V–VI layered compounds Bi_2Te_3, Bi_2Se_3, Sb_2Te_3 and Sb_2Te_2Se, M.R. Thuler, R.L. Benbow and Z. Hurych 71 (1982) 265
Theoretical studies of ion neutralization: two-dimensional tight binding models, H.K. McDowell 72 (1982) 451
An extended Hückel study of hydrogen and oxygen chemisorption on Ru(001) surface, B.C. Khanra and S.K. Saha 76 (1983) 255

Optical activity
Collision-induced absorption in a He–Ar mixture, A. Raczyński 72 (1982) 321
Optical activity of oriented molecules. IX. Phenomenological Mueller matrix description of thick samples and of optical elements, A. Schönhofer, H.-G. Kuball and C. Puebla 76 (1983) 453

Nonlinear optical effects
Fermi-coupled spherically adapted effective states in the collisionless multiphoton excitation of SF_6, C. de Lauro and F. Lattanzi 71 (1982) 233
Interpretation of resonance CARS and Shpolskii spectra with calculated molecular geometries, vibrational frequencies and relative intensities: chrysene in its lowest excited singlet and triplet state, Ch. Jung, A. Lau, H.-J. Weigmann, W. Werncke and M. Pfeiffer 72 (1982) 327
Influence of the molecular environment in solution measurements of the second-order optical susceptibility for urea and derivatives, I. Ledoux and J. Zyss 73 (1982) 203
The polarization dependence of two-photon absorption rates for randomly oriented molecules, M.A.C. Nascimento 74 (1983) 51
Classical aspects of the laser excitation of a Morse oscillator, S.K. Gray 75 (1983) 67
Resonant non-linear spectroscopy in strong fields, B. Dick and R.M. Hochstrasser 75 (1983) 133
Study of IR multiple-photon absorption (MPA) of CF_3Br, E. Borsella, D. Masci, M. Capitelli and M. Dilonardo 77 (1983) 401
Deuterium separation and infrared photochemistry in CF_2HCl, J. Moser, P. Morand, R. Duperrex and H. van den Bergh 79 (1983) 277
Intensity dependence of CO_2-laser-induced multiphoton absorption and decomposition of monomethylamine, D.K. Evans, R.D. McAlpine, H.M. Adams and A.L. Creagh 80 (1983) 379

Field anisotropy
The shape of the Lorentz cavity and the internal field in anisotropic fluids, D.A. Dunmur and R.W. Munn 76 (1983) 249

Transport of charge and mass
The fluctuating-force formulation of friction drag coefficients, J.M. Schurr 71 (1982) 101
Non-hydrodynamic contribution to the concentration dependence of the self diffusion of interacting brownian macroparticles, G.D.J. Phillies 74 (1983) 197
Chemical effects in diffusion and structure of zinc chloride in aqueous solution, A.J. Easteal, P.V. Giaquinta, N.H. March and M.P. Tosi 76 (1983) 125
Polarization energy of a localized charge in a molecular crystal. V. Effect of vacancies, I. Eisenstein and R.W. Munn 77 (1983) 47
Inhibition of Ps formation in benzene and cyclohexane by CH_3Cl and CH_3Br. Correlation to radiation chemistry results, G. Wikander, O.E. Mogensen and N.-J. Pedersen 77 (1983) 159
Comparisons between experimental argon and Lennard-Jones 12:6 shear viscosities, D. Fincham and D.M. Heyes 78 (1983) 425
Quasi-elastic light scattering studies on T7 DNA in the presence of a sinusoidal electric field, K.S. Schmitz 79 (1983) 297

Thermodynamic properties
Electron affinities of higher molybdenum fluorides as determined by the effusion technique, L.N. Sidorov, A.Ya. Borshchevsky, E.B. Rudny and V.D. Butsky 71 (1982) 145
The dissociation energies of gaseous SmLi, EuLi, TmLi and YbLi, A. Neubert and K.F. Zmbov 76 (1983) 469

The determination of thermal conductivity coefficients of liquids by a thermal lens technique, R.T. Bailey, F.R. Cruickshank, D. Pugh, S. Guthrie, A. McLeod, W.S. Foulds, W.R. Lee and S. Venkatesh 77 (1983) 243
Ab initio study of the thermodynamic and kinetic stability of the ammonium radical, H. Cardy, D. Liotard, A. Dargelos and E. Poquet 77 (1983) 287
On the Ne–Ne potential-energy curve and related properties, R.A. Aziz, W.J. Meath and A.R. Allnatt 78 (1983) 295
Theory of sorption of gases on polymers. II. Effects of inter-chain secondary bonds, M. Pyda and M. Kurzyński 79 (1983) 219
Influence of box shape on the hard-disk pressure at high fluid density, W. Schreiner and K.W. Kratky 80 (1983) 245

Structure of solids and liquids
Use of computer simulation to determine the triplet distribution function in dense fluids, S. Gupta, J.M. Haile and W.A. Steele 72 (1982) 425
Satellites in the X-ray photoelectron spectra of transition-metal and rare-earth compounds, D.D. Sarma, P. Vishnu Kamath and C.N.R. Rao 73 (1982) 71
On the structure and dynamics of liquid benzene, O. Steinhauser 73 (1982) 155
Studies of oriented Langmuir–Blodgett multilayers by infrared linear dichroism, P.-A. Chollet and J. Messier 73 (1982) 235
Chiral discrimination in the liquid state: a hard-core model for the rôle of repulsive forces, D.P. Craig and I.R. Elsum 73 (1982) 349
X-ray structure and optical properties of silver films prepared by condensation of preformed Ag-clusters, W. Vogel, B. Tesche and W. Schulze 74 (1983) 137
A crystal orbital investigation on the one-dimensional bis(glyoximato)pyrazine–iron system, M.C. Böhm 76 (1983) 1
Chemical effects in diffusion and structure of zinc chloride in aqueous solution, A.J. Easteal, P.V. Giaquinta, N.H. March and M.P. Tosi 76 (1983) 125
Spectroscopic investigation of the electronic structure of the chlorine molecule in the VUV, Th. Moeller, B. Jordan, P. Gürtler, G. Zimmerer, D. Haaks, J. le Calve and M.-C. Castex 76 (1983) 295
Neutron scattering study of the reorientational motions in $Cr(CO)_3(\eta^6 C_6H_6)$ and $Mn(CO)_3(\eta^5 C_5H_5)$, G. Lucazeau, K. Chhor, C. Sourisseau and A.J. Dianoux 76 (1983) 307
The temperature dependence of the structure of water, P.A. Egelstaff and J.H. Root 76 (1983) 405
Ab initio studies on hydrogen-bonded chains. III. The linear, infinite chain of hydrogen cyanide molecules, A. Karpfen 79 (1983) 211

Phase transitions
Evidence for the existence of structure in gas-phase homomolecular clusters of water, V. Hermann, B.D. Kay and A.W. Castleman Jr. 72 (1982) 185
Diamagnetic anisotropy of molecular complexes of 1,3,5-trinitrobenzene with anthracene and carbazole, R. Burzyński and T. Luty 72 (1982) 441
Computer simulation studies of anisotropic systems. IX. The Maier–Saupe theory for nematic liquid crystals and the molecular field approximation, G.R. Luckhurst, S. Romano and P. Simpson 73 (1982) 337
Acoustic study of a critical binary mixture of nitrobenzene and *n*-hexane at low and ultrasonic frequencies, H. Tanaka, Y. Wada and H. Nakajima 75 (1983) 37
Adiabatic compressibility of critical binary mixtures of nitroethane/isooctane and nitroethane/3-methylpentane, H. Tanaka and Y. Wada 78 (1983) 143

INFORMATION TO AUTHORS

Papers in all areas of Chemical Physics are welcomed, but referees will be asked to judge whether experimental papers have been brought into sufficient relation with theory, and whether theoretical papers bear on experimental verification or exhibit progress in experimental developments to this end.

Contributions written in clear English should be sent *in triplicate* to one of the editors. Contributions may also be submitted to a member of the Advisory Editorial Board who is familiar with the research, in which case *two copies plus the original figures* should be sent simultaneously to one of the editors. In any event, all manuscripts will be refereed at the discretion of the editors.

Authors from the Americas, the Far East and Australia should submit their papers to the American editor; those from Europe, the Near and Middle East and Africa should deal with the European editor.

Manuscripts submitted should be first copies (or clear Xerox copies thereof) typed with double spacing and wide margins; all pages should be numbered, and the text arranged into paragraphs. Before mailing the manuscripts, please check the following points:

1. *Title*: The title should be chosen for its sufficient information content such that it conveys to the informed reader the particular nature of the contents he can expect from the paper. When the length exceeds 45 letters, an abbreviated running title should be indicated.
2. *Abstract*: The abstract of 100–150 words should contain all the substance of the methods and the results achieved as well as keywords of the paper.
3. *Address*: The name(s) of the author(s) and the name and address of the institute, where the research work was done should be indicated on the manuscript. Proofs will be sent by the publisher to this address, unless specifically requested otherwise.
4. *Figures*: The drawings for the figures must be submitted on separate sheets, drawn in black India ink in large size and carefully lettered (with the use of stencils). The lettering as well as the details should have proportionate dimensions so as not to become illegible or unclear after the usual reduction by the printers; in general the figures should be designed for a reduction factor of two or three. Each figure should have a number and a caption; the captions should be collected on a separate sheet. The appropriate place of a figure should be indicated in the margin. Your figure material will be returned after publication of the article.
5. *Formulae*: Displayed formulae should be numbered and typed or clearly written by hand. Vectors will be printed in bold-face italics (heavy, slanting type), and should be indicated by a wavy underlining in the type-script.

   Special attention should be paid to characters that can easily be misread, such as i (lower case), I (cap.), l (el), 1 (one), ′ (prime), o (lower case), O (cap.), 0 (zero), ° (degree), u, v (vee), ν (Greek nu), V (cap.), x, χ, X, z, Z, p, P, ρ (Greek rho), etc.
6. *Tables*: Tables should be typed on separate sheets. Each table should have a number and a title. The appropriate places for the insertion of the tables should be indicated in the margin.
7. *References*: In the text, reference to other parts of the paper should be made by section (or equation) number, not by page number. References to other papers should be consecutively numbered in the text and should be listed by number, preferably as in the following examples:

   For a book: A. Messiah, Quantum mechanics, Vol. 1 (North-Holland, Amsterdam, 1970).

   For a paper in a journal: C.J. Winscom and A.H. Maki, Chem. Phys. Letters 12 (1971) 264.

   For a paper in a contributed volume: A. Carrington, in: Magnetic resonance and radiofrequency spectroscopy, ed. P. Averbuch (North-Holland, Amsterdam, 1968) p. 23.

   For an unpublished paper: G.J. Lycett, Ph.D. Thesis, University of Birmingham, England (1970).
8. *Footnotes*: As far as possible, footnotes should be avoided.

Upon acceptance of an article by the journal, author(s) will be asked to transfer copyright of the article to the publisher. This transfer will ensure the widest possible dissemination of information.

Now available in paperback!

Stochastic Processes in Physics and Chemistry

by N. G. VAN KAMPEN, *University of Utrecht, Utrecht, The Netherlands*

1981 (1st. repr. 1983) xiv + 416 pages **Price: US $28.00/Dfl. 75.00** ISBN 0-444-86200-5

This is what **PHYSICS TODAY** had to say about this important work, now available in paperback, which first appeared in 1981:-

"... van Kampen has produced a superbly written, physically motivated introduction to the theory of stochastic processes. ...an excellent introduction to the use (and avoidance of abuse) of master equations. It should be in every physics and chemistry library."

The interest in fluctuations and in the stochastic method for describing them has grown enormously in the last few decades. The number of articles scattered in the literature of various disciplines must run to thousands and special journals are devoted to the subject. Yet the physicist or chemist who wants to become acquainted with the field cannot easily find a suitable introduction. This book is an attempt to fill this gap in the literature.

The first part consists of an introductory exposition of probability, random events, and stochastic processes as they occur in physics, chemistry and biology, in particular, Markov processes and their master equation. The emphasis is on applications rather than mathematics. Subsequently, approximation methods are developed for obtaining relevant information for nonlinear systems. A discussion of unstable and spatially continuous systems will prepare the reader for the rapidly developing literature on these subjects. The final chapter introduces stochastic differential equations. There are numerous exercises throughout the book.

CONTENTS: Preface. *Chapters:* I. Stochastic Variables. II. Random Events. III. Stochastic Processes. IV. Markov Processes. V. The Master Equation. VI. One-Step Processes. VII. Chemical Reactions. VIII. The Fokker-Planck and Langevin Equations. IX. The Expansion of the Master Equation. X. The Diffusion Type. XI. Unstable Systems. XII. Fluctuations in Continuous Systems. XIII. The Statistics of Jump Events. XIV. Stochastic Differential Equations. Index.

NORTH-HOLLAND

IN THE U.S.A. AND CANADA:
ELSEVIER SCIENCE PUBLISHING CO., INC.
P.O. BOX 1663
GRAND CENTRAL STATION
NEW YORK, NY 10163

IN ALL OTHER COUNTRIES:
ELSEVIER SCIENCE PUBLISHERS
P.O. BOX 211
1000 AE AMSTERDAM
THE NETHERLANDS

US $ prices are valid only in the USA and Canada. In all other countries the Dutch Guilder price is definitive. All prices are subject to change without prior notice.

p1543 NH